



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:37 AM GMT

PDB ID : 1KLF
Title : FIMH ADHESIN-FIMC CHAPERONE COMPLEX WITH D-MANNOSE
Authors : Hung, C.S.; Bouckaert, J.
Deposited on : 2001-12-11
Resolution : 2.79 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

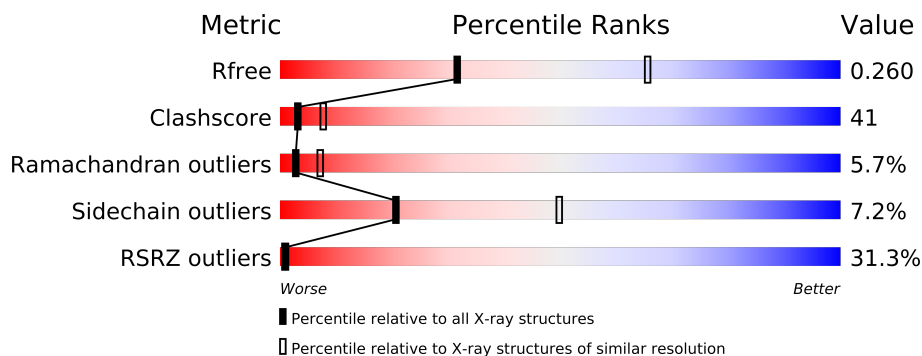
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	205	
1	C	205	
1	E	205	
1	G	205	
1	I	205	
1	K	205	
1	M	205	
1	O	205	
2	B	279	
2	D	279	
2	F	279	
2	H	279	
2	J	279	
2	L	279	

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Mol	Chain	Length	Quality of chain
2	N	279	
2	P	279	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29775 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CHAPERONE PROTEIN FIMC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	C	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	E	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	G	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	I	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	K	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	M	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			
1	O	205	Total	C	N	O	S	0	0	0
			1596	1010	276	304	6			

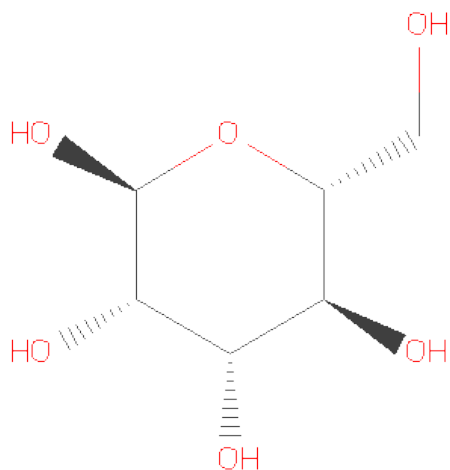
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	VAL	GLU	CONFLICT	UNP P31697
C	18	VAL	GLU	CONFLICT	UNP P31697
E	18	VAL	GLU	CONFLICT	UNP P31697
G	18	VAL	GLU	CONFLICT	UNP P31697
I	18	VAL	GLU	CONFLICT	UNP P31697
K	18	VAL	GLU	CONFLICT	UNP P31697
M	18	VAL	GLU	CONFLICT	UNP P31697
O	18	VAL	GLU	CONFLICT	UNP P31697

- Molecule 2 is a protein called FIMH PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	D	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	F	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	H	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	J	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	L	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	N	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			
2	P	279	Total	C	N	O	S	0	0	0
			2052	1297	342	409	4			

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			12	6	6		
3	J	1	Total	C	O	0	0
			12	6	6		
3	N	1	Total	C	O	0	0
			12	6	6		
3	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	82	Total	O	0	0
			82	82		
4	C	37	Total	O	0	0
			37	37		
4	D	69	Total	O	0	0
			69	69		
4	E	39	Total	O	0	0
			39	39		
4	F	78	Total	O	0	0
			78	78		
4	G	39	Total	O	0	0
			39	39		
4	H	73	Total	O	0	0
			73	73		
4	I	2	Total	O	0	0
			2	2		
4	J	9	Total	O	0	0
			9	9		
4	K	4	Total	O	0	0
			4	4		
4	L	8	Total	O	0	0
			8	8		
4	M	2	Total	O	0	0
			2	2		
4	N	8	Total	O	0	0
			8	8		
4	O	4	Total	O	0	0
			4	4		

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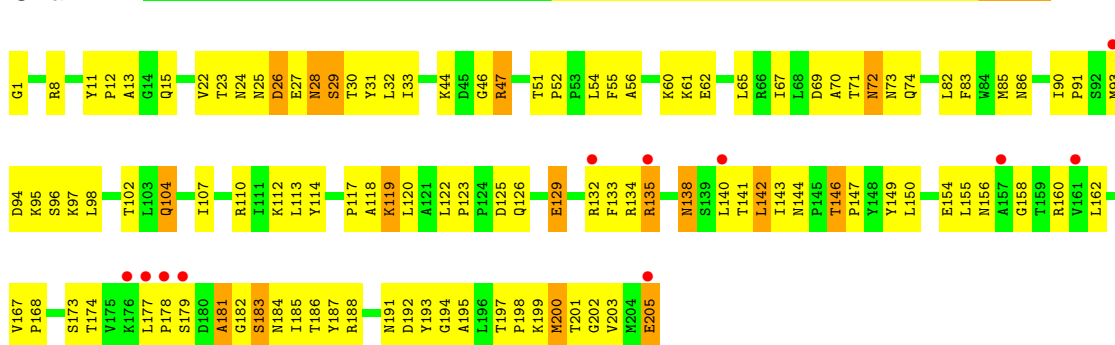
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	7	Total	O	0	0
			7	7		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

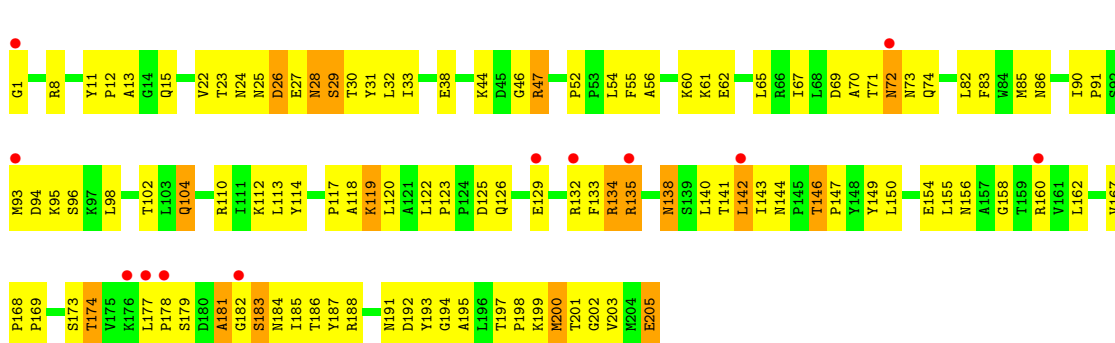
• Molecule 1: CHAPERONE PROTEIN FIMC

Chain A:



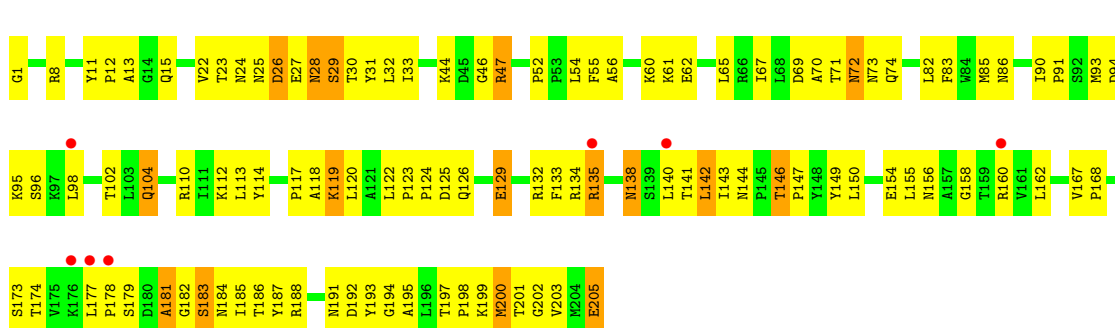
• Molecule 1: CHAPERONE PROTEIN FIMC

Chain C:



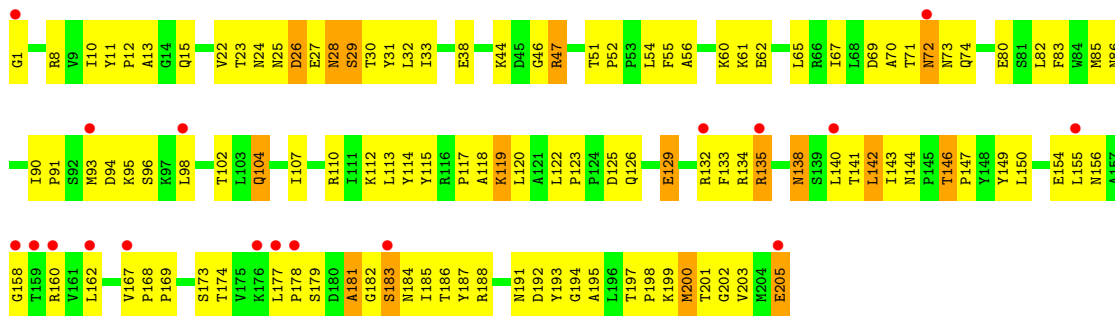
• Molecule 1: CHAPERONE PROTEIN FIMC

Chain E:



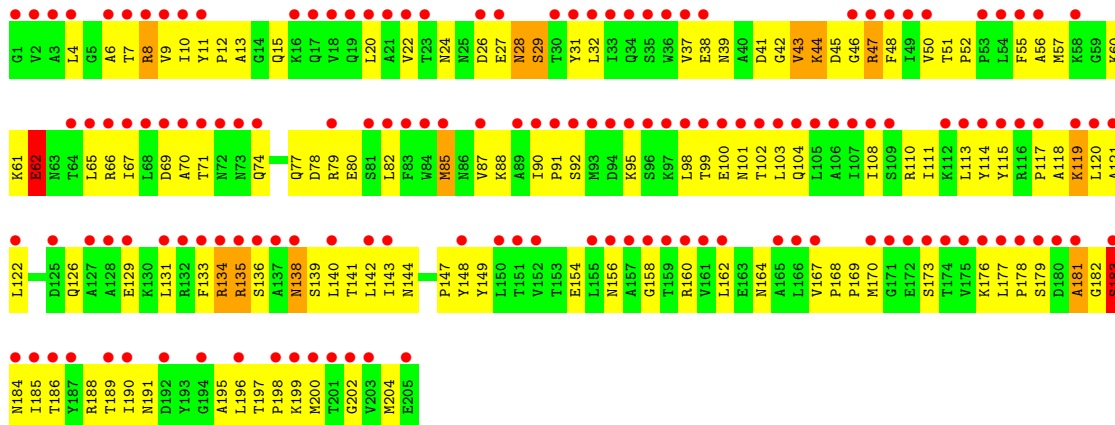
- Molecule 1: CHAPERONE PROTEIN FIMC

Chain G:



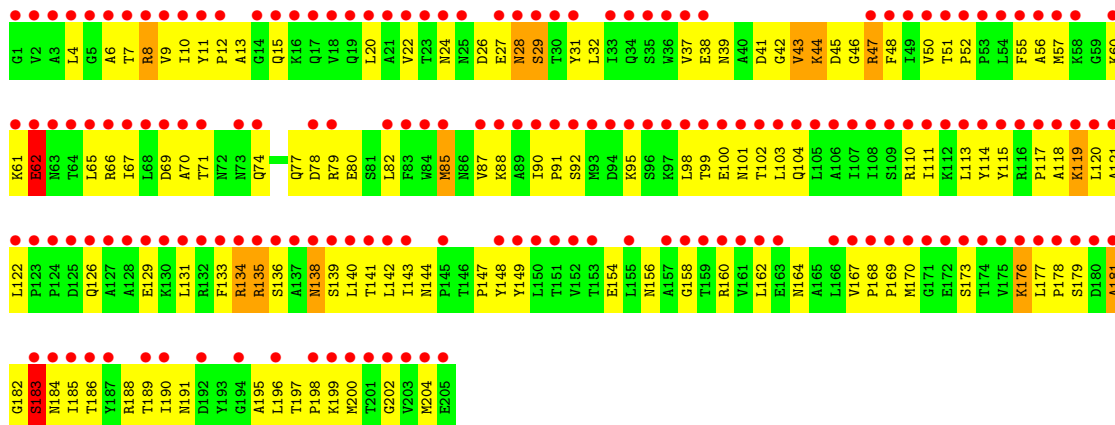
- Molecule 1: CHAPERONE PROTEIN FIMC

Chain I:



- Molecule 1: CHAPERONE PROTEIN FIMC

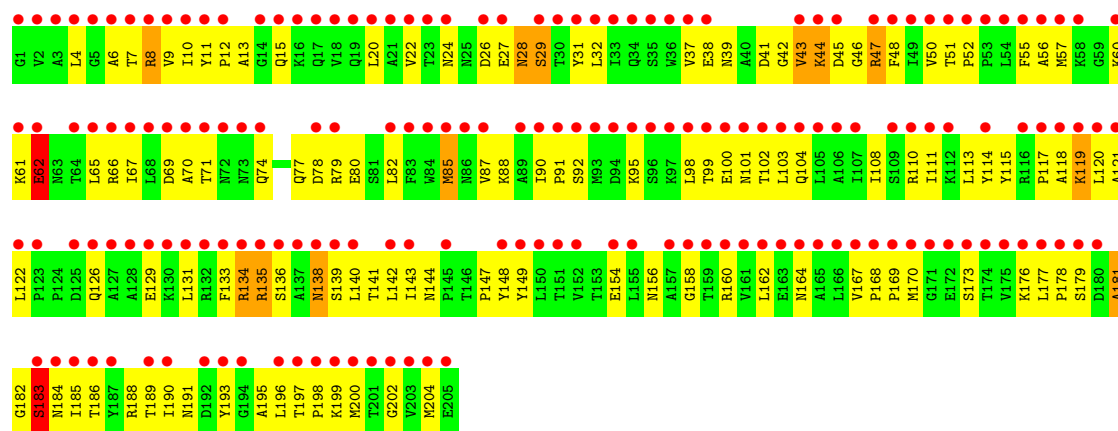
Chain K:



- Molecule 1: CHAPERONE PROTEIN FIMC

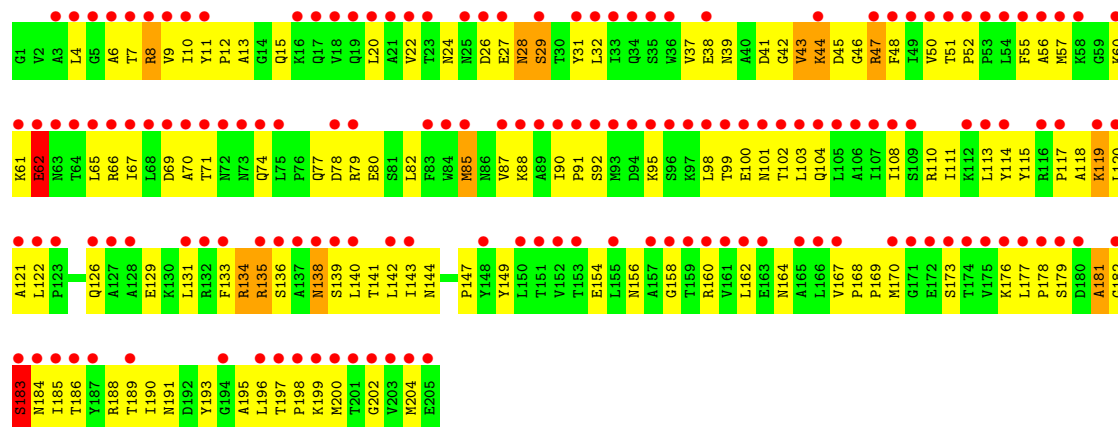
Chain M:





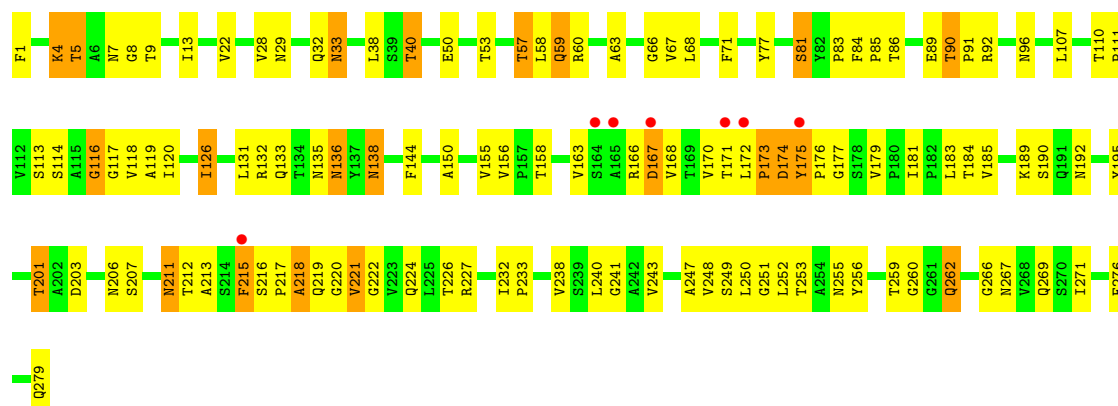
• Molecule 1: CHAPERONE PROTEIN FIMC

Chain O:



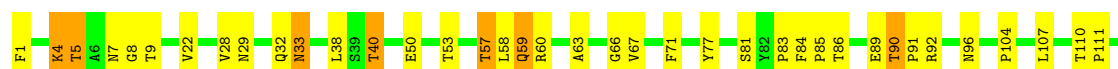
• Molecule 2: FIMH PROTEIN

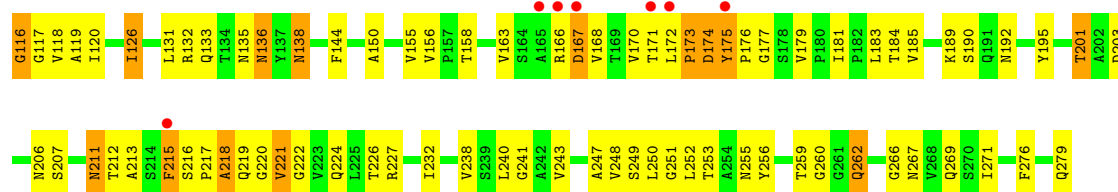
Chain B:



• Molecule 2: FIMH PROTEIN

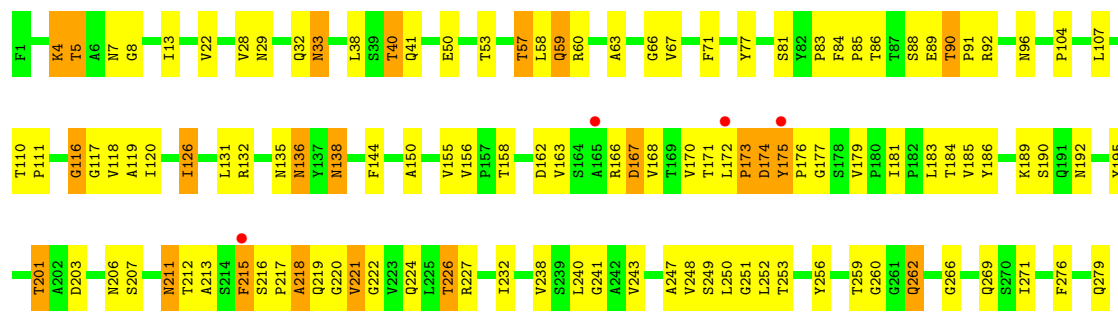
Chain D:





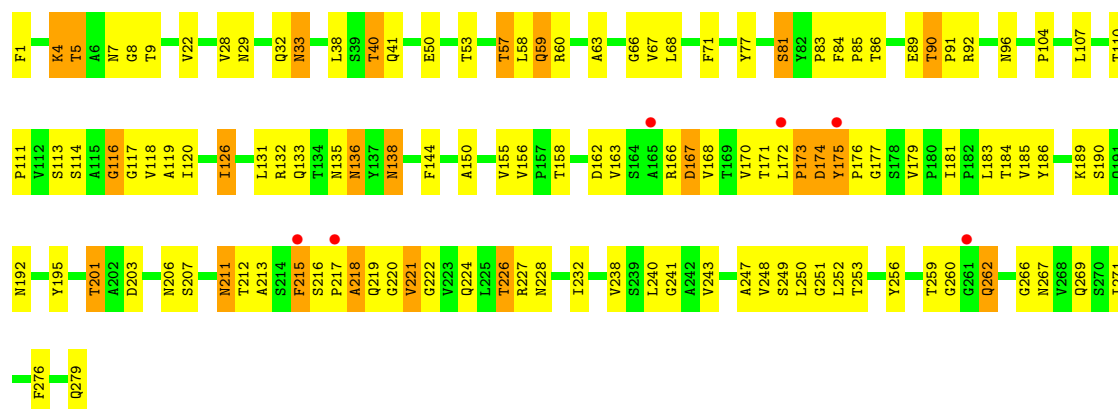
• Molecule 2: FIMH PROTEIN

Chain F: 



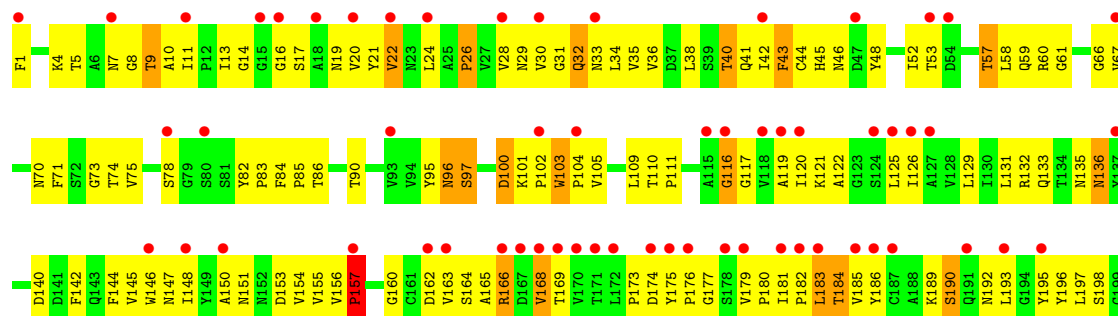
• Molecule 2: FIMH PROTEIN

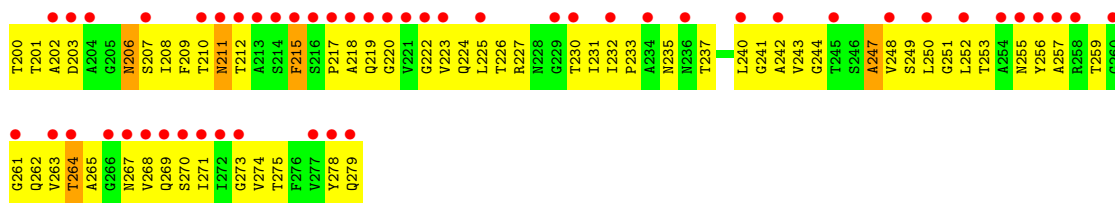
Chain H: 



• Molecule 2: FIMH PROTEIN

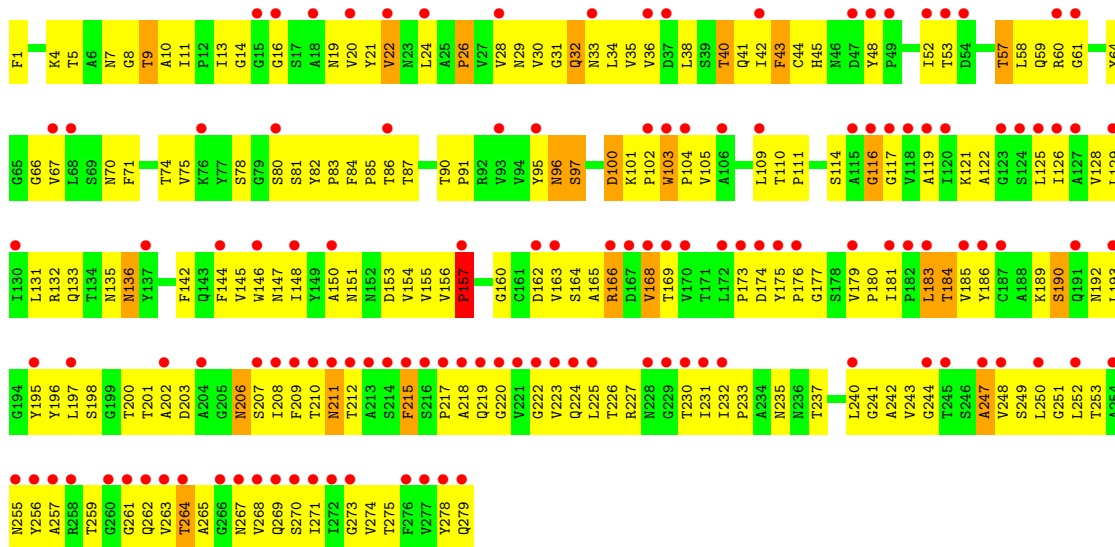
Chain J: 





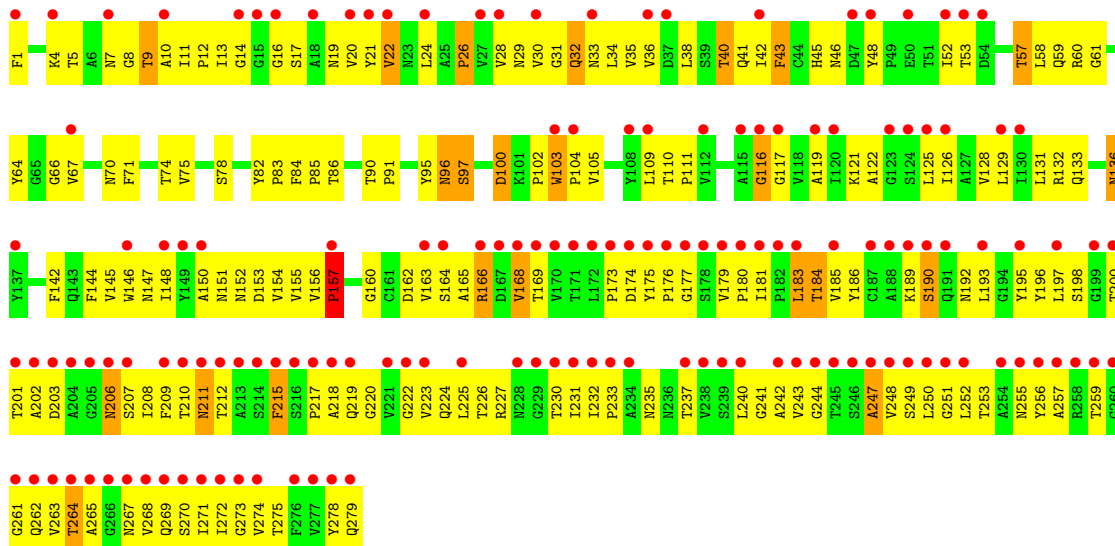
• Molecule 2: FIMH PROTEIN

Chain L:



• Molecule 2: FIMH PROTEIN

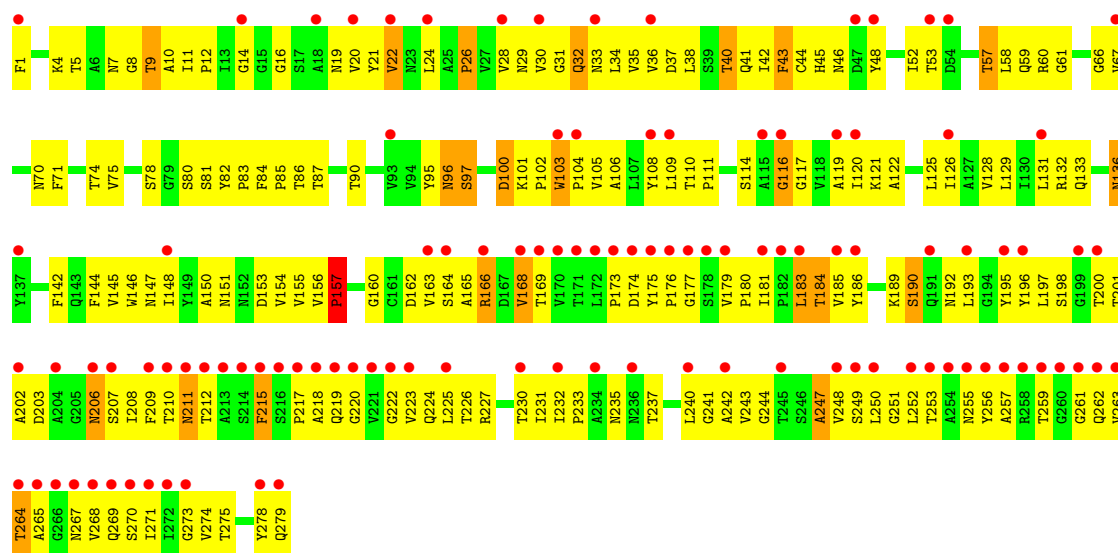
Chain N:



• Molecule 2: FIMH PROTEIN

Chain P:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.08Å 138.13Å 215.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.79 43.68 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.68-2.79) 99.0 (43.68-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.280 0.240 , 0.260	Depositor DCC
R_{free} test set	9936 reflections (11.14%)	DCC
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.1	EDS
Estimated twinning fraction	0.477 for k,h,-l 0.476 for -k,-h,-l 0.477 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 99135 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29775	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/1625	0.74	0/2209
1	C	0.42	0/1625	0.74	0/2209
1	E	0.42	0/1625	0.73	0/2209
1	G	0.42	0/1625	0.74	0/2209
1	I	0.29	0/1625	0.58	0/2209
1	K	0.29	0/1625	0.59	0/2209
1	M	0.29	0/1625	0.59	0/2209
1	O	0.29	0/1625	0.59	0/2209
2	B	0.48	0/2097	0.76	0/2881
2	D	0.48	0/2097	0.76	0/2881
2	F	0.48	0/2097	0.76	0/2881
2	H	0.48	0/2097	0.76	0/2881
2	J	0.31	0/2097	0.59	0/2881
2	L	0.31	0/2097	0.59	0/2881
2	N	0.31	0/2097	0.59	0/2881
2	P	0.31	0/2097	0.59	0/2881
All	All	0.38	0/29776	0.67	0/40720

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1639	133	0
1	C	1596	0	1639	142	0
1	E	1596	0	1639	125	0
1	G	1596	0	1639	135	0
1	I	1596	0	1639	149	0
1	K	1596	0	1639	149	0
1	M	1596	0	1639	152	0
1	O	1596	0	1639	152	0
2	B	2052	0	2007	141	0
2	D	2052	0	2007	142	0
2	F	2052	0	2007	135	0
2	H	2052	0	2007	141	0
2	J	2052	0	2007	200	0
2	L	2052	0	2007	205	0
2	N	2052	0	2007	203	0
2	P	2052	0	2007	208	0
3	B	12	0	12	0	0
3	D	12	0	12	0	0
3	F	12	0	12	0	0
3	H	12	0	12	0	0
3	J	12	0	12	4	0
3	L	12	0	12	2	0
3	N	12	0	12	1	0
3	P	12	0	12	2	0
4	A	34	0	0	3	0
4	B	82	0	0	3	0
4	C	37	0	0	1	0
4	D	69	0	0	4	0
4	E	39	0	0	0	0
4	F	78	0	0	4	0
4	G	39	0	0	3	0
4	H	73	0	0	4	0
4	I	2	0	0	0	0
4	J	9	0	0	1	0
4	K	4	0	0	0	0
4	L	8	0	0	1	0
4	M	2	0	0	0	0
4	N	8	0	0	0	0
4	O	4	0	0	0	0
4	P	7	0	0	0	0
All	All	29775	0	29264	2407	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (2407) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:134:ARG:HB3	1:C:141:THR:HG22	1.26	1.14
2:P:224:GLN:HE21	2:P:231:ILE:HG21	1.16	1.10
2:F:126:ILE:HD12	2:F:150:ALA:HB2	1.33	1.10
2:H:126:ILE:HD12	2:H:150:ALA:HB2	1.34	1.09
2:D:126:ILE:HD12	2:D:150:ALA:HB2	1.33	1.09
2:J:224:GLN:HE21	2:J:231:ILE:HG21	1.17	1.08
2:B:126:ILE:HD12	2:B:150:ALA:HB2	1.33	1.07
2:L:201:THR:HG21	2:L:206:ASN:HA	1.38	1.06
2:N:224:GLN:HE21	2:N:231:ILE:HG21	1.17	1.05
2:L:196:TYR:HE1	2:L:198:SER:HB3	1.22	1.05
2:J:196:TYR:HE1	2:J:198:SER:HB3	1.21	1.05
2:L:224:GLN:HE21	2:L:231:ILE:HG21	1.17	1.04
2:N:196:TYR:HE1	2:N:198:SER:HB3	1.22	1.03
2:N:201:THR:HG21	2:N:206:ASN:HA	1.37	1.03
2:J:201:THR:HG21	2:J:206:ASN:HA	1.38	1.03
2:P:196:TYR:HE1	2:P:198:SER:HB3	1.22	1.00
2:B:201:THR:HG21	2:B:206:ASN:HA	1.44	1.00
2:P:201:THR:HG21	2:P:206:ASN:HA	1.38	1.00
2:H:201:THR:HG21	2:H:206:ASN:HA	1.44	1.00
2:D:201:THR:HG21	2:D:206:ASN:HA	1.44	0.99
2:F:201:THR:HG21	2:F:206:ASN:HA	1.45	0.98
1:C:134:ARG:HB3	1:C:141:THR:CG2	1.93	0.98
1:M:47:ARG:HH22	1:M:74:GLN:HE21	1.08	0.97
2:B:170:VAL:HG12	2:B:172:LEU:HB2	1.47	0.97
2:D:170:VAL:HG12	2:D:172:LEU:HB2	1.47	0.96
1:K:47:ARG:HH22	1:K:74:GLN:HE21	1.07	0.96
1:O:47:ARG:HH22	1:O:74:GLN:HE21	1.07	0.96
2:F:120:ILE:HG21	2:F:126:ILE:HD11	1.48	0.96
2:F:170:VAL:HG12	2:F:172:LEU:HB2	1.47	0.96
2:H:170:VAL:HG12	2:H:172:LEU:HB2	1.47	0.95
2:H:5:THR:HG21	4:H:1644:HOH:O	1.68	0.94
2:N:202:ALA:HB2	2:N:210:THR:HG22	1.50	0.94
2:L:57:THR:HG23	2:L:132:ARG:HB3	1.48	0.94
2:P:202:ALA:HB2	2:P:210:THR:HG22	1.50	0.94
2:D:213:ALA:HB2	2:D:269:GLN:HB2	1.50	0.93
2:L:202:ALA:HB2	2:L:210:THR:HG22	1.50	0.93
1:C:47:ARG:HH22	1:C:74:GLN:HE21	0.99	0.93
2:J:202:ALA:HB2	2:J:210:THR:HG22	1.50	0.93
1:E:47:ARG:HH22	1:E:74:GLN:HE21	0.98	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:135:ARG:HH12	1:G:181:ALA:HB1	1.34	0.93
2:B:120:ILE:HG21	2:B:126:ILE:HD11	1.49	0.92
2:D:120:ILE:HG21	2:D:126:ILE:HD11	1.49	0.92
2:N:57:THR:HG23	2:N:132:ARG:HB3	1.48	0.92
2:J:57:THR:HG23	2:J:132:ARG:HB3	1.49	0.92
1:I:47:ARG:HH22	1:I:74:GLN:HE21	1.07	0.92
2:P:57:THR:HG23	2:P:132:ARG:HB3	1.50	0.92
2:H:120:ILE:HG21	2:H:126:ILE:HD11	1.49	0.92
1:G:47:ARG:HH22	1:G:74:GLN:HE21	0.98	0.92
2:F:57:THR:HG22	2:F:132:ARG:HB3	1.52	0.92
2:P:264:THR:HG22	2:P:265:ALA:H	1.35	0.91
1:C:135:ARG:HH12	1:C:181:ALA:HB1	1.33	0.91
1:M:39:ASN:HD21	1:M:43:VAL:HG13	1.35	0.91
2:L:67:VAL:HG21	2:L:126:ILE:HG23	1.51	0.91
2:H:57:THR:HG22	2:H:132:ARG:HB3	1.50	0.91
2:J:264:THR:HG22	2:J:265:ALA:H	1.35	0.91
1:K:39:ASN:HD21	1:K:43:VAL:HG13	1.36	0.91
2:N:163:VAL:HA	2:N:185:VAL:HG22	1.53	0.91
1:A:47:ARG:HH22	1:A:74:GLN:HE21	0.96	0.91
2:L:163:VAL:HA	2:L:185:VAL:HG22	1.52	0.91
1:G:179:SER:C	1:G:181:ALA:H	1.74	0.91
1:A:135:ARG:HH12	1:A:181:ALA:HB1	1.34	0.91
2:H:213:ALA:HB2	2:H:269:GLN:HB2	1.52	0.91
2:N:67:VAL:HG21	2:N:126:ILE:HG23	1.52	0.91
1:E:135:ARG:HH12	1:E:181:ALA:HB1	1.34	0.90
2:J:163:VAL:HA	2:J:185:VAL:HG22	1.53	0.90
2:P:67:VAL:HG21	2:P:126:ILE:HG23	1.51	0.90
2:L:264:THR:HG22	2:L:265:ALA:H	1.35	0.90
1:I:39:ASN:HD21	1:I:43:VAL:HG13	1.36	0.90
1:E:179:SER:C	1:E:181:ALA:H	1.74	0.89
2:J:67:VAL:HG21	2:J:126:ILE:HG23	1.51	0.89
2:P:163:VAL:HA	2:P:185:VAL:HG22	1.52	0.89
1:A:179:SER:C	1:A:181:ALA:H	1.74	0.89
2:F:213:ALA:HB2	2:F:269:GLN:HB2	1.52	0.89
2:N:264:THR:HG22	2:N:265:ALA:H	1.36	0.89
2:B:57:THR:HG21	2:B:89:GLU:OE2	1.73	0.89
1:O:39:ASN:HD21	1:O:43:VAL:HG13	1.36	0.89
2:B:213:ALA:HB2	2:B:269:GLN:HB2	1.53	0.89
2:F:57:THR:HG21	2:F:89:GLU:OE2	1.72	0.89
2:H:167:ASP:CG	2:H:168:VAL:H	1.77	0.88
2:B:167:ASP:CG	2:B:168:VAL:H	1.76	0.88
1:A:133:PHE:HD2	1:A:140:LEU:HD21	1.38	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:57:THR:HG21	2:H:89:GLU:OE2	1.73	0.88
1:M:135:ARG:NH1	1:M:181:ALA:HB1	1.89	0.88
1:C:179:SER:C	1:C:181:ALA:H	1.75	0.88
1:I:176:LYS:H	1:I:176:LYS:HD2	1.38	0.88
1:O:135:ARG:NH1	1:O:181:ALA:HB1	1.89	0.87
1:I:27:GLU:HG2	1:I:60:LYS:HD2	1.55	0.87
1:C:133:PHE:HD2	1:C:140:LEU:HD21	1.39	0.87
2:B:57:THR:HG22	2:B:132:ARG:HB3	1.57	0.87
1:K:134:ARG:HB3	1:K:141:THR:HB	1.56	0.87
1:K:176:LYS:HD2	1:K:176:LYS:H	1.38	0.87
1:M:176:LYS:HD2	1:M:176:LYS:H	1.39	0.87
1:K:135:ARG:NH1	1:K:181:ALA:HB1	1.89	0.86
1:M:27:GLU:HG2	1:M:60:LYS:HD2	1.55	0.86
1:I:134:ARG:HB3	1:I:141:THR:HB	1.56	0.86
1:E:138:ASN:HA	1:E:177:LEU:O	1.76	0.86
2:N:11:ILE:HG23	2:N:16:GLY:HA3	1.57	0.86
1:E:133:PHE:HD2	1:E:140:LEU:HD21	1.38	0.86
1:I:135:ARG:NH1	1:I:181:ALA:HB1	1.89	0.86
1:O:27:GLU:HG2	1:O:60:LYS:HD2	1.55	0.86
2:D:167:ASP:CG	2:D:168:VAL:H	1.76	0.86
1:O:134:ARG:HB3	1:O:141:THR:HB	1.56	0.86
1:C:138:ASN:HA	1:C:177:LEU:O	1.76	0.86
1:G:133:PHE:HD2	1:G:140:LEU:HD21	1.39	0.86
2:D:57:THR:HG21	2:D:89:GLU:OE2	1.75	0.86
2:D:57:THR:HG22	2:D:132:ARG:HB3	1.56	0.86
1:K:27:GLU:HG2	1:K:60:LYS:HD2	1.55	0.86
2:J:58:LEU:H	2:J:90:THR:CG2	1.89	0.86
2:P:11:ILE:HG23	2:P:16:GLY:HA3	1.56	0.85
2:J:11:ILE:HG23	2:J:16:GLY:HA3	1.56	0.85
1:O:135:ARG:HH12	1:O:181:ALA:CB	1.90	0.85
1:G:138:ASN:HA	1:G:177:LEU:O	1.76	0.85
1:M:134:ARG:HB3	1:M:141:THR:HB	1.56	0.85
2:D:92:ARG:HH11	2:D:92:ARG:HG3	1.41	0.85
2:P:58:LEU:H	2:P:90:THR:CG2	1.90	0.85
2:P:58:LEU:H	2:P:90:THR:HG22	1.42	0.85
1:A:138:ASN:HA	1:A:177:LEU:O	1.76	0.84
2:J:5:THR:HG22	2:J:7:ASN:H	1.42	0.84
2:B:92:ARG:HG3	2:B:92:ARG:HH11	1.40	0.84
1:O:176:LYS:H	1:O:176:LYS:HD2	1.38	0.84
2:P:196:TYR:CE1	2:P:198:SER:HB3	2.11	0.84
2:L:11:ILE:HG23	2:L:16:GLY:HA3	1.56	0.84
1:C:135:ARG:HH12	1:C:181:ALA:CB	1.89	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:ARG:HH12	1:E:181:ALA:CB	1.90	0.84
2:P:5:THR:HG22	2:P:7:ASN:H	1.43	0.84
1:K:135:ARG:HH12	1:K:181:ALA:CB	1.91	0.84
1:G:135:ARG:HH12	1:G:181:ALA:CB	1.90	0.84
1:M:135:ARG:HH12	1:M:181:ALA:CB	1.90	0.84
2:F:167:ASP:CG	2:F:168:VAL:H	1.76	0.84
2:J:196:TYR:CE1	2:J:198:SER:HB3	2.11	0.84
2:N:196:TYR:CE1	2:N:198:SER:HB3	2.11	0.84
1:I:135:ARG:HH12	1:I:181:ALA:CB	1.91	0.84
2:H:59:GLN:HG2	2:H:132:ARG:HD2	1.60	0.83
2:L:58:LEU:H	2:L:90:THR:HG22	1.42	0.83
2:L:196:TYR:CE1	2:L:198:SER:HB3	2.11	0.83
1:A:135:ARG:HH12	1:A:181:ALA:CB	1.90	0.83
1:C:135:ARG:NH1	1:C:181:ALA:HB1	1.93	0.83
2:N:5:THR:HG22	2:N:7:ASN:H	1.42	0.83
2:J:58:LEU:H	2:J:90:THR:HG22	1.41	0.83
2:N:58:LEU:H	2:N:90:THR:CG2	1.91	0.83
2:L:5:THR:HG22	2:L:7:ASN:H	1.43	0.83
2:B:59:GLN:HG2	2:B:132:ARG:HD2	1.60	0.83
2:L:58:LEU:H	2:L:90:THR:CG2	1.90	0.83
1:G:141:THR:OG1	1:G:174:THR:HG22	1.78	0.82
1:E:47:ARG:NH2	1:E:74:GLN:HE21	1.76	0.82
2:D:192:ASN:HD22	2:D:279:GLN:HE22	1.26	0.82
2:L:226:THR:HB	2:L:231:ILE:HG12	1.62	0.82
2:F:92:ARG:HH11	2:F:92:ARG:HG3	1.44	0.82
1:A:47:ARG:NH2	1:A:74:GLN:HE21	1.75	0.82
2:H:92:ARG:HG3	2:H:92:ARG:HH11	1.42	0.82
2:P:226:THR:HB	2:P:231:ILE:HG12	1.62	0.82
2:N:58:LEU:H	2:N:90:THR:HG22	1.42	0.82
2:N:224:GLN:NE2	2:N:231:ILE:HG21	1.95	0.82
2:H:192:ASN:HD22	2:H:279:GLN:HE22	1.27	0.82
1:G:47:ARG:NH2	1:G:74:GLN:HE21	1.76	0.82
2:F:59:GLN:HG2	2:F:132:ARG:HD2	1.60	0.82
2:D:53:THR:H	2:D:136:ASN:HD21	1.27	0.82
1:I:177:LEU:HD12	1:I:178:PRO:HD2	1.61	0.81
2:N:253:THR:HG22	2:N:255:ASN:HD21	1.45	0.81
1:O:177:LEU:HD12	1:O:178:PRO:HD2	1.61	0.81
2:J:253:THR:HG22	2:J:255:ASN:HD21	1.44	0.81
2:P:34:LEU:HD12	2:P:35:VAL:H	1.44	0.81
2:B:192:ASN:HD22	2:B:279:GLN:HE22	1.26	0.81
2:N:34:LEU:HD12	2:N:35:VAL:H	1.45	0.81
2:D:59:GLN:HG2	2:D:132:ARG:HD2	1.60	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:8:ARG:HB3	1:I:8:ARG:NH2	1.95	0.81
1:M:8:ARG:NH2	1:M:8:ARG:HB3	1.95	0.81
2:P:224:GLN:NE2	2:P:231:ILE:HG21	1.94	0.81
2:P:253:THR:HG22	2:P:255:ASN:HD21	1.45	0.81
1:E:135:ARG:NH1	1:E:181:ALA:HB1	1.94	0.81
2:H:53:THR:H	2:H:136:ASN:HD21	1.27	0.81
1:A:135:ARG:NH1	1:A:181:ALA:HB1	1.94	0.81
2:F:53:THR:H	2:F:136:ASN:HD21	1.26	0.81
2:L:253:THR:HG22	2:L:255:ASN:HD21	1.45	0.81
1:M:177:LEU:HD12	1:M:178:PRO:HD2	1.61	0.81
1:G:135:ARG:NH1	1:G:181:ALA:HB1	1.94	0.81
1:K:177:LEU:HD12	1:K:178:PRO:HD2	1.61	0.81
2:B:53:THR:H	2:B:136:ASN:HD21	1.26	0.81
2:N:208:ILE:HG23	2:N:257:ALA:HB1	1.63	0.81
2:L:34:LEU:HD12	2:L:35:VAL:H	1.45	0.80
1:M:39:ASN:ND2	1:M:43:VAL:HG13	1.95	0.80
1:I:39:ASN:ND2	1:I:43:VAL:HG13	1.96	0.80
2:D:218:ALA:HB2	2:D:266:GLY:C	2.02	0.80
2:F:218:ALA:HB2	2:F:266:GLY:C	2.02	0.80
2:P:208:ILE:HG23	2:P:257:ALA:HB1	1.64	0.80
2:J:226:THR:HB	2:J:231:ILE:HG12	1.62	0.80
1:M:8:ARG:HH21	1:M:8:ARG:HB3	1.47	0.80
2:L:208:ILE:HG23	2:L:257:ALA:HB1	1.63	0.80
1:K:39:ASN:ND2	1:K:43:VAL:HG13	1.96	0.80
1:O:39:ASN:ND2	1:O:43:VAL:HG13	1.96	0.80
1:O:8:ARG:NH2	1:O:8:ARG:HB3	1.95	0.80
1:M:32:LEU:HB2	1:M:90:ILE:HB	1.64	0.80
2:H:218:ALA:HB2	2:H:266:GLY:C	2.02	0.79
2:J:224:GLN:NE2	2:J:231:ILE:HG21	1.95	0.79
2:J:208:ILE:HG23	2:J:257:ALA:HB1	1.64	0.79
2:B:218:ALA:HB2	2:B:266:GLY:C	2.02	0.79
2:N:226:THR:HB	2:N:231:ILE:HG12	1.62	0.79
1:K:47:ARG:NH2	1:K:74:GLN:HE21	1.81	0.79
1:E:47:ARG:HG3	1:E:71:THR:HB	1.65	0.79
1:I:47:ARG:NH2	1:I:74:GLN:HE21	1.81	0.79
2:J:34:LEU:HD12	2:J:35:VAL:H	1.45	0.79
1:K:8:ARG:HB3	1:K:8:ARG:NH2	1.96	0.79
1:O:47:ARG:NH2	1:O:74:GLN:HE21	1.81	0.79
2:F:192:ASN:HD22	2:F:279:GLN:HE22	1.31	0.79
2:L:224:GLN:NE2	2:L:231:ILE:HG21	1.95	0.79
1:K:32:LEU:HB2	1:K:90:ILE:HB	1.64	0.79
1:C:47:ARG:NH2	1:C:74:GLN:HE21	1.78	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:38:GLU:HG2	1:M:44:LYS:HG3	1.65	0.78
1:G:52:PRO:HG2	1:G:55:PHE:CD2	2.18	0.78
1:I:8:ARG:HB3	1:I:8:ARG:HH21	1.47	0.78
2:N:21:TYR:HB3	2:N:151:ASN:HD21	1.49	0.78
1:O:32:LEU:HB2	1:O:90:ILE:HB	1.64	0.78
1:E:188:ARG:HH11	1:E:199:LYS:HB2	1.49	0.78
2:N:59:GLN:HG3	2:N:132:ARG:HB2	1.66	0.78
1:O:8:ARG:HH21	1:O:8:ARG:HB3	1.47	0.78
1:G:188:ARG:HH11	1:G:199:LYS:HB2	1.49	0.78
1:G:47:ARG:HG3	1:G:71:THR:HB	1.65	0.78
1:A:188:ARG:HH11	1:A:199:LYS:HB2	1.48	0.78
2:D:192:ASN:HD22	2:D:279:GLN:NE2	1.82	0.78
1:A:47:ARG:HG3	1:A:71:THR:HB	1.64	0.77
1:K:38:GLU:HG2	1:K:44:LYS:HG3	1.65	0.77
1:C:52:PRO:HG2	1:C:55:PHE:CD2	2.19	0.77
1:C:134:ARG:HD2	1:C:141:THR:CG2	2.14	0.77
2:P:226:THR:HG23	2:P:253:THR:HB	1.67	0.77
2:N:226:THR:HG23	2:N:253:THR:HB	1.66	0.77
1:M:47:ARG:NH2	1:M:74:GLN:HE21	1.81	0.77
1:O:38:GLU:HG2	1:O:44:LYS:HG3	1.65	0.77
2:J:226:THR:HG23	2:J:253:THR:HB	1.66	0.77
1:C:47:ARG:HG3	1:C:71:THR:HB	1.65	0.77
2:P:21:TYR:HB3	2:P:151:ASN:HD21	1.50	0.77
2:D:172:LEU:O	2:D:174:ASP:N	2.18	0.77
1:I:32:LEU:HB2	1:I:90:ILE:HB	1.64	0.77
2:L:226:THR:HG23	2:L:253:THR:HB	1.67	0.77
2:B:192:ASN:HD22	2:B:279:GLN:NE2	1.83	0.77
2:J:21:TYR:HB3	2:J:151:ASN:HD21	1.49	0.77
1:C:134:ARG:HD2	1:C:141:THR:HG21	1.67	0.76
2:L:59:GLN:HG3	2:L:132:ARG:HB2	1.67	0.76
1:K:8:ARG:HB3	1:K:8:ARG:HH21	1.47	0.76
2:L:21:TYR:HB3	2:L:151:ASN:HD21	1.50	0.76
2:H:172:LEU:O	2:H:174:ASP:N	2.18	0.76
2:J:59:GLN:HG3	2:J:132:ARG:HB2	1.66	0.76
1:O:176:LYS:HD2	1:O:176:LYS:N	2.00	0.76
1:K:52:PRO:HG2	1:K:55:PHE:CD2	2.20	0.76
2:P:197:LEU:HD13	2:P:225:LEU:HD12	1.67	0.76
2:B:172:LEU:O	2:B:174:ASP:N	2.18	0.76
2:P:59:GLN:HG3	2:P:132:ARG:HB2	1.67	0.76
1:O:52:PRO:HG2	1:O:55:PHE:CD2	2.21	0.76
1:A:32:LEU:HB2	1:A:90:ILE:HB	1.68	0.76
1:C:32:LEU:HB2	1:C:90:ILE:HB	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:172:LEU:O	2:F:174:ASP:N	2.18	0.76
1:C:188:ARG:HH11	1:C:199:LYS:HB2	1.49	0.76
1:E:52:PRO:HG2	1:E:55:PHE:CD2	2.21	0.75
1:I:52:PRO:HG2	1:I:55:PHE:CD2	2.20	0.75
1:G:112:LYS:HG3	4:G:209:HOH:O	1.86	0.75
1:I:38:GLU:HG2	1:I:44:LYS:HG3	1.65	0.75
1:M:52:PRO:HG2	1:M:55:PHE:CD2	2.21	0.75
1:A:52:PRO:HG2	1:A:55:PHE:CD2	2.21	0.75
2:L:197:LEU:HD13	2:L:225:LEU:HD12	1.68	0.75
2:B:173:PRO:HG3	2:B:179:VAL:HG13	1.69	0.75
1:A:47:ARG:HH22	1:A:74:GLN:NE2	1.80	0.75
1:O:185:ILE:HB	1:O:202:GLY:HA3	1.68	0.75
1:K:176:LYS:HD2	1:K:176:LYS:N	2.00	0.75
2:P:180:PRO:HA	2:P:253:THR:HA	1.70	0.74
2:J:197:LEU:HD13	2:J:225:LEU:HD12	1.67	0.74
2:N:197:LEU:HD13	2:N:225:LEU:HD12	1.68	0.74
1:I:185:ILE:HB	1:I:202:GLY:HA3	1.68	0.74
1:M:185:ILE:HB	1:M:202:GLY:HA3	1.68	0.74
1:G:32:LEU:HB2	1:G:90:ILE:HB	1.69	0.74
2:H:192:ASN:HD22	2:H:279:GLN:NE2	1.85	0.74
2:D:173:PRO:HG3	2:D:179:VAL:HG13	1.69	0.74
1:C:134:ARG:CB	1:C:141:THR:HG22	2.15	0.74
2:N:180:PRO:HA	2:N:253:THR:HA	1.70	0.74
2:H:171:THR:C	2:H:173:PRO:HD2	2.08	0.74
1:E:32:LEU:HB2	1:E:90:ILE:HB	1.70	0.74
1:K:185:ILE:HB	1:K:202:GLY:HA3	1.68	0.74
1:E:47:ARG:HH22	1:E:74:GLN:NE2	1.82	0.73
2:L:180:PRO:HA	2:L:253:THR:HA	1.70	0.73
2:H:173:PRO:HG3	2:H:179:VAL:HG13	1.70	0.73
2:L:180:PRO:HB3	2:L:253:THR:HG23	1.71	0.73
2:F:171:THR:C	2:F:173:PRO:HD2	2.08	0.73
1:M:176:LYS:HD2	1:M:176:LYS:N	2.00	0.73
2:P:180:PRO:HB3	2:P:253:THR:HG23	1.71	0.73
1:A:110:ARG:HD3	4:A:222:HOH:O	1.87	0.73
2:B:171:THR:C	2:B:173:PRO:HD2	2.08	0.73
1:G:47:ARG:HH22	1:G:74:GLN:NE2	1.82	0.73
2:D:226:THR:HG23	4:D:1618:HOH:O	1.88	0.73
2:L:186:TYR:HB3	2:L:247:ALA:HA	1.71	0.73
2:D:29:ASN:HD22	2:D:32:GLN:HE22	1.37	0.73
2:J:180:PRO:HA	2:J:253:THR:HA	1.70	0.73
2:N:180:PRO:HB3	2:N:253:THR:HG23	1.71	0.73
2:F:29:ASN:HD22	2:F:32:GLN:HE22	1.36	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:19:ASN:HD21	2:P:219:GLN:NE2	1.85	0.73
2:H:29:ASN:HD22	2:H:32:GLN:HE22	1.36	0.73
1:M:111:ILE:HG22	2:N:278:TYR:HB2	1.72	0.72
2:J:19:ASN:HD21	2:L:219:GLN:NE2	1.87	0.72
2:F:173:PRO:HG3	2:F:179:VAL:HG13	1.70	0.72
2:N:186:TYR:HB3	2:N:247:ALA:HA	1.71	0.72
2:J:180:PRO:HB3	2:J:253:THR:HG23	1.72	0.72
2:D:201:THR:HG21	2:D:206:ASN:HD22	1.55	0.72
2:H:57:THR:CG2	2:H:132:ARG:HB3	2.19	0.72
2:H:29:ASN:HD22	2:H:32:GLN:NE2	1.88	0.72
1:M:101:ASN:HD22	2:N:268:VAL:HG23	1.55	0.72
2:B:29:ASN:HD22	2:B:32:GLN:HE22	1.37	0.72
1:C:141:THR:HB	1:C:174:THR:HG23	1.72	0.72
1:A:112:LYS:HG3	4:A:208:HOH:O	1.90	0.72
1:I:176:LYS:N	1:I:176:LYS:HD2	2.00	0.71
2:P:186:TYR:HB3	2:P:247:ALA:HA	1.71	0.71
1:O:101:ASN:HD22	2:P:268:VAL:HG23	1.56	0.71
2:F:29:ASN:HD22	2:F:32:GLN:NE2	1.87	0.71
1:O:111:ILE:HG22	2:P:278:TYR:HB2	1.72	0.71
2:F:192:ASN:HD22	2:F:279:GLN:NE2	1.87	0.71
1:C:141:THR:O	1:C:141:THR:HG23	1.90	0.71
2:F:201:THR:HG21	2:F:206:ASN:HD22	1.54	0.71
2:J:186:TYR:HB3	2:J:247:ALA:HA	1.71	0.71
2:D:29:ASN:HD22	2:D:32:GLN:NE2	1.89	0.71
2:H:262:GLN:HE21	2:H:262:GLN:HA	1.56	0.71
2:B:201:THR:HG21	2:B:206:ASN:HD22	1.56	0.71
2:D:171:THR:C	2:D:173:PRO:HD2	2.10	0.71
1:C:47:ARG:HH22	1:C:74:GLN:NE2	1.83	0.71
2:F:57:THR:CG2	2:F:132:ARG:HB3	2.21	0.71
2:D:32:GLN:O	2:D:110:THR:HG23	1.91	0.71
2:J:48:TYR:HB2	2:J:52:ILE:HD12	1.73	0.71
1:I:111:ILE:HG22	2:J:278:TYR:HB2	1.72	0.71
2:B:29:ASN:HD22	2:B:32:GLN:NE2	1.89	0.71
2:H:32:GLN:O	2:H:110:THR:HG23	1.90	0.70
2:P:155:VAL:HG12	2:P:157:PRO:HD3	1.73	0.70
2:D:173:PRO:HB2	2:D:177:GLY:HA3	1.73	0.70
2:B:32:GLN:O	2:B:110:THR:HG23	1.91	0.70
2:N:155:VAL:HG12	2:N:157:PRO:HD3	1.73	0.70
1:K:101:ASN:HD22	2:L:268:VAL:HG23	1.56	0.70
1:K:111:ILE:HG22	2:L:278:TYR:HB2	1.72	0.70
1:I:101:ASN:HD22	2:J:268:VAL:HG23	1.56	0.70
1:M:12:PRO:HB2	1:M:15:GLN:HG2	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:201:THR:HG21	2:H:206:ASN:HD22	1.55	0.70
2:L:164:SER:HB2	2:L:184:THR:HG23	1.74	0.70
2:B:262:GLN:HA	2:B:262:GLN:HE21	1.56	0.70
1:M:182:GLY:O	1:M:183:SER:HB2	1.92	0.70
2:P:48:TYR:HB2	2:P:52:ILE:HD12	1.74	0.70
2:F:32:GLN:O	2:F:110:THR:HG23	1.91	0.69
2:N:48:TYR:HB2	2:N:52:ILE:HD12	1.74	0.69
2:F:262:GLN:HA	2:F:262:GLN:HE21	1.56	0.69
2:D:57:THR:CG2	2:D:132:ARG:HB3	2.22	0.69
1:I:12:PRO:HB2	1:I:15:GLN:HG2	1.73	0.69
1:E:12:PRO:HG2	1:E:15:GLN:HE21	1.57	0.69
2:B:173:PRO:HB2	2:B:177:GLY:HA3	1.74	0.69
2:F:218:ALA:HB2	2:F:266:GLY:O	1.93	0.69
2:N:164:SER:HB2	2:N:184:THR:HG23	1.75	0.69
2:B:81:SER:O	2:P:114:SER:HB2	1.92	0.69
1:O:162:LEU:HD21	1:O:178:PRO:HD3	1.75	0.69
1:K:162:LEU:HD21	1:K:178:PRO:HD3	1.75	0.69
1:K:12:PRO:HB2	1:K:15:GLN:HG2	1.73	0.69
1:O:12:PRO:HB2	1:O:15:GLN:HG2	1.73	0.69
2:H:58:LEU:H	2:H:90:THR:HG22	1.57	0.69
2:F:172:LEU:N	2:F:173:PRO:HD2	2.07	0.69
1:I:162:LEU:HD21	1:I:178:PRO:HD3	1.75	0.69
1:G:25:ASN:O	1:G:60:LYS:HG2	1.93	0.69
2:L:48:TYR:HB2	2:L:52:ILE:HD12	1.73	0.69
2:D:262:GLN:HE21	2:D:262:GLN:HA	1.57	0.69
2:D:172:LEU:N	2:D:173:PRO:HD2	2.08	0.69
2:H:173:PRO:HB2	2:H:177:GLY:HA3	1.74	0.69
2:H:172:LEU:N	2:H:173:PRO:HD2	2.06	0.69
1:C:25:ASN:O	1:C:60:LYS:HG2	1.93	0.69
1:E:112:LYS:HG3	4:F:1506:HOH:O	1.92	0.69
2:J:155:VAL:HG12	2:J:157:PRO:HD3	1.73	0.69
1:I:182:GLY:O	1:I:183:SER:HB2	1.93	0.69
2:L:155:VAL:HG12	2:L:157:PRO:HD3	1.73	0.69
1:C:141:THR:CB	1:C:174:THR:HG23	2.22	0.69
2:J:264:THR:HG22	2:J:265:ALA:N	2.08	0.69
1:O:88:LYS:HE2	1:O:90:ILE:HG12	1.75	0.69
2:P:164:SER:HB2	2:P:184:THR:HG23	1.75	0.69
1:I:82:LEU:HD13	1:I:114:TYR:CE2	2.28	0.69
1:C:12:PRO:HB2	1:C:15:GLN:CG	2.23	0.69
2:L:264:THR:HG22	2:L:265:ALA:N	2.08	0.68
1:M:162:LEU:HD21	1:M:178:PRO:HD3	1.75	0.68
1:M:88:LYS:HE2	1:M:90:ILE:HG12	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:164:SER:HB2	2:J:184:THR:HG23	1.74	0.68
1:A:12:PRO:HB2	1:A:15:GLN:CG	2.22	0.68
1:C:182:GLY:O	1:C:183:SER:HB2	1.92	0.68
2:B:172:LEU:N	2:B:173:PRO:HD2	2.07	0.68
1:C:112:LYS:HG3	4:D:1605:HOH:O	1.94	0.68
2:H:81:SER:O	2:L:114:SER:HB2	1.93	0.68
1:A:182:GLY:O	1:A:183:SER:HB2	1.92	0.68
1:G:182:GLY:O	1:G:183:SER:HB2	1.93	0.68
1:A:12:PRO:HG2	1:A:15:GLN:HE21	1.58	0.68
2:B:57:THR:CG2	2:B:132:ARG:HB3	2.24	0.68
2:B:218:ALA:HB2	2:B:266:GLY:O	1.94	0.68
1:M:82:LEU:HD13	1:M:114:TYR:CE2	2.28	0.68
1:O:82:LEU:HD13	1:O:114:TYR:CE2	2.28	0.68
1:E:86:ASN:HD21	1:E:110:ARG:HE	1.42	0.68
1:G:86:ASN:HD21	1:G:110:ARG:HE	1.41	0.68
2:H:53:THR:HB	2:H:136:ASN:OD1	1.93	0.68
2:D:218:ALA:HB2	2:D:266:GLY:O	1.93	0.68
1:G:12:PRO:HG2	1:G:15:GLN:HE21	1.59	0.68
1:O:135:ARG:NH1	1:O:181:ALA:CB	2.53	0.68
1:G:27:GLU:HG3	1:G:60:LYS:HD2	1.74	0.68
2:F:173:PRO:HB2	2:F:177:GLY:HA3	1.74	0.68
1:E:182:GLY:O	1:E:183:SER:HB2	1.93	0.68
1:K:79:ARG:HB3	1:K:170:MET:CE	2.24	0.68
1:M:138:ASN:HA	1:M:177:LEU:O	1.94	0.68
1:K:135:ARG:NH1	1:K:181:ALA:CB	2.53	0.68
2:B:116:GLY:HA2	2:B:189:LYS:HE2	1.76	0.68
1:A:25:ASN:O	1:A:60:LYS:HG2	1.93	0.68
1:C:12:PRO:HG2	1:C:15:GLN:HE21	1.59	0.68
1:K:82:LEU:HD13	1:K:114:TYR:CE2	2.29	0.68
2:D:53:THR:HB	2:D:136:ASN:OD1	1.94	0.67
1:K:88:LYS:HE2	1:K:90:ILE:HG12	1.76	0.67
1:G:12:PRO:HB2	1:G:15:GLN:CG	2.24	0.67
1:I:79:ARG:HB3	1:I:170:MET:CE	2.24	0.67
1:O:79:ARG:HB3	1:O:170:MET:CE	2.23	0.67
2:B:53:THR:H	2:B:136:ASN:ND2	1.92	0.67
1:A:86:ASN:HD21	1:A:110:ARG:HE	1.42	0.67
1:A:144:ASN:ND2	1:A:150:LEU:HG	2.10	0.67
1:K:138:ASN:HA	1:K:177:LEU:O	1.94	0.67
1:I:138:ASN:HA	1:I:177:LEU:O	1.94	0.67
2:F:58:LEU:H	2:F:90:THR:HG22	1.59	0.67
1:K:182:GLY:O	1:K:183:SER:HB2	1.93	0.67
2:N:105:VAL:HG11	2:N:129:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:24:LEU:HD22	2:P:36:VAL:HG22	1.77	0.67
1:E:25:ASN:O	1:E:60:LYS:HG2	1.93	0.67
2:B:58:LEU:H	2:B:90:THR:HG22	1.58	0.67
2:B:226:THR:HG23	4:B:1508:HOH:O	1.94	0.67
1:O:138:ASN:HA	1:O:177:LEU:O	1.94	0.67
1:G:188:ARG:NH1	1:G:199:LYS:H	1.92	0.67
2:J:186:TYR:HB2	2:J:244:GLY:O	1.95	0.67
1:O:12:PRO:HB2	1:O:15:GLN:CG	2.25	0.67
2:B:217:PRO:O	2:B:219:GLN:N	2.28	0.67
2:D:221:VAL:O	2:D:259:THR:HG23	1.95	0.67
2:B:53:THR:HB	2:B:136:ASN:OD1	1.94	0.67
2:N:219:GLN:OE1	2:N:262:GLN:HG2	1.95	0.67
2:H:211:ASN:HD22	2:H:212:THR:N	1.92	0.67
2:D:53:THR:H	2:D:136:ASN:ND2	1.93	0.67
1:E:27:GLU:HG3	1:E:60:LYS:HD2	1.74	0.67
1:C:86:ASN:HD21	1:C:110:ARG:HE	1.42	0.67
2:D:116:GLY:HA2	2:D:189:LYS:HE2	1.77	0.67
1:O:182:GLY:O	1:O:183:SER:HB2	1.93	0.67
2:H:218:ALA:HB2	2:H:266:GLY:O	1.93	0.67
1:A:12:PRO:HB2	1:A:15:GLN:HG3	1.77	0.67
1:C:188:ARG:NH1	1:C:199:LYS:H	1.92	0.67
1:A:188:ARG:NH1	1:A:199:LYS:H	1.93	0.67
1:I:88:LYS:HE2	1:I:90:ILE:HG12	1.75	0.67
1:M:79:ARG:HB3	1:M:170:MET:CE	2.24	0.67
2:N:24:LEU:HD22	2:N:36:VAL:HG22	1.77	0.66
1:M:135:ARG:CZ	1:M:181:ALA:HB1	2.25	0.66
1:C:27:GLU:HG3	1:C:60:LYS:HD2	1.75	0.66
1:A:27:GLU:HG3	1:A:60:LYS:HD2	1.76	0.66
1:E:188:ARG:NH1	1:E:199:LYS:H	1.94	0.66
2:P:219:GLN:OE1	2:P:262:GLN:HG2	1.95	0.66
2:N:186:TYR:HB2	2:N:244:GLY:O	1.95	0.66
1:C:12:PRO:HB2	1:C:15:GLN:HG3	1.77	0.66
2:H:84:PHE:HA	2:H:85:PRO:C	2.15	0.66
2:P:264:THR:HG22	2:P:265:ALA:N	2.07	0.66
1:I:135:ARG:CZ	1:I:181:ALA:HB1	2.25	0.66
1:M:126:GLN:HA	1:M:129:GLU:OE1	1.96	0.66
2:H:217:PRO:O	2:H:219:GLN:N	2.28	0.66
1:M:12:PRO:HB2	1:M:15:GLN:CG	2.25	0.66
2:H:77:TYR:CD2	2:H:90:THR:HG21	2.30	0.66
1:C:110:ARG:HD3	4:C:223:HOH:O	1.95	0.66
1:C:122:LEU:HD11	1:C:126:GLN:O	1.95	0.66
2:N:264:THR:HG22	2:N:265:ALA:N	2.08	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:219:GLN:OE1	2:L:262:GLN:HG2	1.94	0.66
2:P:186:TYR:HB2	2:P:244:GLY:O	1.96	0.66
2:L:24:LEU:HD22	2:L:36:VAL:HG22	1.76	0.66
2:F:211:ASN:HD22	2:F:212:THR:N	1.93	0.66
1:O:135:ARG:CZ	1:O:181:ALA:HB1	2.25	0.66
1:I:102:THR:O	2:J:269:GLN:HA	1.96	0.66
2:D:217:PRO:O	2:D:219:GLN:N	2.29	0.66
1:I:10:ILE:O	1:I:12:PRO:HD3	1.96	0.66
1:K:103:LEU:HD12	2:L:270:SER:O	1.96	0.66
2:J:219:GLN:OE1	2:J:262:GLN:HG2	1.94	0.66
2:B:221:VAL:O	2:B:259:THR:HG23	1.96	0.66
2:F:116:GLY:HA2	2:F:189:LYS:HE2	1.77	0.66
1:M:135:ARG:NH1	1:M:181:ALA:CB	2.53	0.66
1:I:12:PRO:HB2	1:I:15:GLN:CG	2.25	0.66
1:C:144:ASN:ND2	1:C:150:LEU:HG	2.10	0.66
2:D:77:TYR:CD2	2:D:90:THR:HG21	2.30	0.66
1:K:126:GLN:HA	1:K:129:GLU:OE1	1.95	0.66
2:L:43:PHE:CD2	2:L:102:PRO:HB3	2.31	0.66
2:H:53:THR:H	2:H:136:ASN:ND2	1.94	0.65
2:D:58:LEU:H	2:D:90:THR:HG22	1.60	0.65
2:N:43:PHE:CD2	2:N:102:PRO:HB3	2.31	0.65
1:G:12:PRO:HB2	1:G:15:GLN:HG3	1.78	0.65
1:O:79:ARG:HB3	1:O:170:MET:HE1	1.79	0.65
2:P:43:PHE:CD2	2:P:102:PRO:HB3	2.31	0.65
1:A:122:LEU:HD11	1:A:126:GLN:O	1.96	0.65
1:M:102:THR:O	2:N:269:GLN:HA	1.96	0.65
1:I:103:LEU:HD12	2:J:270:SER:O	1.96	0.65
2:J:24:LEU:HD22	2:J:36:VAL:HG22	1.77	0.65
1:O:126:GLN:HA	1:O:129:GLU:OE1	1.96	0.65
1:K:135:ARG:CZ	1:K:181:ALA:HB1	2.25	0.65
1:K:12:PRO:HB2	1:K:15:GLN:CG	2.25	0.65
1:O:10:ILE:O	1:O:12:PRO:HD3	1.96	0.65
1:I:126:GLN:HA	1:I:129:GLU:OE1	1.95	0.65
2:L:116:GLY:HA3	2:L:189:LYS:HG3	1.79	0.65
1:G:73:ASN:HA	4:G:222:HOH:O	1.97	0.65
2:F:53:THR:HB	2:F:136:ASN:OD1	1.95	0.65
2:B:77:TYR:CD2	2:B:90:THR:HG21	2.31	0.65
1:G:144:ASN:ND2	1:G:150:LEU:HG	2.12	0.65
2:F:53:THR:H	2:F:136:ASN:ND2	1.93	0.65
1:I:79:ARG:HB3	1:I:170:MET:HE1	1.78	0.65
2:N:116:GLY:HA3	2:N:189:LYS:HG3	1.79	0.65
2:L:105:VAL:HG11	2:L:129:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:122:LEU:HD11	1:E:126:GLN:O	1.97	0.65
1:O:102:THR:O	2:P:269:GLN:HA	1.96	0.65
2:B:211:ASN:HD22	2:B:212:THR:N	1.94	0.65
1:G:122:LEU:HD11	1:G:126:GLN:O	1.96	0.65
2:J:105:VAL:HG11	2:J:129:LEU:HD13	1.77	0.65
2:F:217:PRO:O	2:F:219:GLN:N	2.30	0.65
2:L:186:TYR:HB2	2:L:244:GLY:O	1.95	0.65
1:E:12:PRO:HB2	1:E:15:GLN:CG	2.26	0.65
2:F:221:VAL:O	2:F:259:THR:HG23	1.96	0.65
1:M:103:LEU:HD12	2:N:270:SER:O	1.96	0.65
1:O:103:LEU:HD12	2:P:270:SER:O	1.96	0.65
1:E:144:ASN:ND2	1:E:150:LEU:HG	2.11	0.65
2:J:58:LEU:N	2:J:90:THR:HG22	2.12	0.65
1:K:10:ILE:O	1:K:12:PRO:HD3	1.96	0.65
1:K:102:THR:O	2:L:269:GLN:HA	1.96	0.65
2:D:84:PHE:HA	2:D:85:PRO:C	2.17	0.65
2:B:90:THR:HG23	2:B:91:PRO:O	1.96	0.64
2:J:84:PHE:HA	2:J:85:PRO:C	2.18	0.64
2:P:105:VAL:HG11	2:P:129:LEU:HD13	1.78	0.64
2:P:95:TYR:OH	2:P:103:TRP:HA	1.97	0.64
2:J:38:LEU:C	2:J:40:THR:H	2.00	0.64
2:F:77:TYR:CD2	2:F:90:THR:HG21	2.31	0.64
2:F:167:ASP:CG	2:F:168:VAL:N	2.50	0.64
2:L:38:LEU:C	2:L:40:THR:H	2.01	0.64
2:P:116:GLY:HA3	2:P:189:LYS:HG3	1.79	0.64
2:D:211:ASN:HD22	2:D:212:THR:N	1.94	0.64
1:M:10:ILE:O	1:M:12:PRO:HD3	1.96	0.64
2:D:90:THR:HG23	2:D:91:PRO:O	1.97	0.64
2:J:43:PHE:CD2	2:J:102:PRO:HB3	2.32	0.64
2:J:116:GLY:HA3	2:J:189:LYS:HG3	1.79	0.64
2:F:84:PHE:HA	2:F:85:PRO:C	2.17	0.64
2:P:58:LEU:N	2:P:90:THR:HG22	2.12	0.64
2:B:192:ASN:ND2	2:B:279:GLN:HE22	1.95	0.64
2:J:43:PHE:HA	2:J:102:PRO:HA	1.80	0.64
2:B:84:PHE:HA	2:B:85:PRO:C	2.16	0.64
2:H:221:VAL:O	2:H:259:THR:HG23	1.97	0.64
1:M:27:GLU:HA	1:M:60:LYS:HG3	1.79	0.64
2:J:95:TYR:OH	2:J:103:TRP:HA	1.97	0.64
2:H:116:GLY:HA2	2:H:189:LYS:HE2	1.79	0.64
1:C:134:ARG:CD	1:C:141:THR:HG21	2.28	0.64
2:N:95:TYR:OH	2:N:103:TRP:HA	1.97	0.64
2:L:43:PHE:HA	2:L:102:PRO:HA	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:102:THR:CA	2:F:171:THR:HG22	2.28	0.64
2:N:43:PHE:HA	2:N:102:PRO:HA	1.80	0.64
1:A:97:LYS:HE3	4:B:1573:HOH:O	1.96	0.64
2:L:67:VAL:HG13	2:L:109:LEU:HD13	1.80	0.63
2:L:84:PHE:HA	2:L:85:PRO:C	2.18	0.63
1:G:102:THR:CA	2:H:171:THR:HG22	2.28	0.63
1:A:156:ASN:HB2	1:A:186:THR:OG1	1.99	0.63
1:A:179:SER:C	1:A:181:ALA:N	2.50	0.63
1:O:135:ARG:NH1	1:O:177:LEU:HD11	2.13	0.63
2:D:167:ASP:CG	2:D:168:VAL:N	2.50	0.63
1:K:27:GLU:HA	1:K:60:LYS:HG3	1.80	0.63
2:L:95:TYR:OH	2:L:103:TRP:HA	1.98	0.63
1:M:4:LEU:HD21	1:M:87:VAL:HG21	1.80	0.63
2:N:67:VAL:HG13	2:N:109:LEU:HD13	1.79	0.63
2:P:38:LEU:C	2:P:40:THR:H	2.01	0.63
1:C:102:THR:CA	2:D:171:THR:HG22	2.27	0.63
1:E:179:SER:C	1:E:181:ALA:N	2.50	0.63
1:M:162:LEU:HD21	1:M:178:PRO:CD	2.29	0.63
2:D:92:ARG:NH1	2:D:92:ARG:HG3	2.10	0.63
2:P:84:PHE:HA	2:P:85:PRO:C	2.17	0.63
1:G:140:LEU:HD23	1:G:141:THR:N	2.14	0.63
2:B:92:ARG:HG3	2:B:92:ARG:NH1	2.09	0.63
2:N:58:LEU:N	2:N:90:THR:HG22	2.13	0.63
2:N:84:PHE:HA	2:N:85:PRO:C	2.18	0.63
1:G:104:GLN:HG3	2:H:168:VAL:HG23	1.81	0.63
1:K:135:ARG:NH1	1:K:177:LEU:HD11	2.13	0.63
2:L:58:LEU:N	2:L:90:THR:HG22	2.13	0.63
1:C:134:ARG:CZ	1:C:141:THR:HG21	2.29	0.63
1:C:11:TYR:HB2	1:C:113:LEU:HD11	1.81	0.63
1:M:27:GLU:CG	1:M:60:LYS:HD2	2.29	0.63
1:O:4:LEU:HD21	1:O:87:VAL:HG21	1.81	0.63
2:F:67:VAL:HG23	2:F:126:ILE:HG12	1.81	0.63
1:A:102:THR:CA	2:B:171:THR:HG22	2.28	0.63
1:G:94:ASP:HB3	1:G:96:SER:OG	1.98	0.63
1:O:162:LEU:HD21	1:O:178:PRO:CD	2.29	0.63
2:J:32:GLN:O	2:J:110:THR:HG23	1.99	0.63
1:G:179:SER:C	1:G:181:ALA:N	2.50	0.62
1:M:135:ARG:NH1	1:M:177:LEU:HD11	2.13	0.62
1:I:27:GLU:HA	1:I:60:LYS:HG3	1.80	0.62
1:O:27:GLU:HA	1:O:60:LYS:HG3	1.80	0.62
2:H:90:THR:HG23	2:H:91:PRO:O	1.98	0.62
1:I:4:LEU:HD21	1:I:87:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:38:LEU:C	2:N:40:THR:H	2.01	0.62
1:A:140:LEU:HD23	1:A:141:THR:N	2.14	0.62
2:P:32:GLN:O	2:P:110:THR:HG23	1.99	0.62
1:C:140:LEU:HD23	1:C:141:THR:N	2.15	0.62
1:C:185:ILE:HB	1:C:202:GLY:HA3	1.81	0.62
1:A:185:ILE:HB	1:A:202:GLY:HA3	1.82	0.62
1:I:135:ARG:NH1	1:I:177:LEU:HD11	2.13	0.62
2:D:192:ASN:ND2	2:D:279:GLN:HE22	1.94	0.62
1:G:185:ILE:HB	1:G:202:GLY:HA3	1.81	0.62
1:E:12:PRO:HB2	1:E:15:GLN:HG3	1.82	0.62
2:D:172:LEU:O	2:D:172:LEU:HD23	1.99	0.62
2:N:59:GLN:CG	2:N:132:ARG:HB2	2.28	0.62
2:J:20:VAL:HG21	2:J:42:ILE:HD11	1.81	0.62
2:N:184:THR:HA	2:N:249:SER:HA	1.81	0.62
1:E:156:ASN:HB2	1:E:186:THR:OG1	2.00	0.62
2:B:59:GLN:CG	2:B:132:ARG:HD2	2.30	0.62
1:G:156:ASN:HB2	1:G:186:THR:OG1	2.00	0.62
2:P:59:GLN:CG	2:P:132:ARG:HB2	2.29	0.62
2:P:43:PHE:HA	2:P:102:PRO:HA	1.79	0.62
2:N:32:GLN:O	2:N:110:THR:HG23	2.00	0.62
1:G:191:ASN:HD21	1:G:195:ALA:HB3	1.64	0.62
2:J:59:GLN:CG	2:J:132:ARG:HB2	2.29	0.62
2:P:67:VAL:HG13	2:P:109:LEU:HD13	1.80	0.62
1:A:94:ASP:HB3	1:A:96:SER:OG	2.00	0.62
1:K:162:LEU:HD21	1:K:178:PRO:CD	2.29	0.62
1:C:94:ASP:HB3	1:C:96:SER:OG	1.99	0.62
2:F:90:THR:HG23	2:F:91:PRO:O	1.98	0.62
1:C:156:ASN:HB2	1:C:186:THR:OG1	2.00	0.62
2:B:170:VAL:CG1	2:B:172:LEU:HB2	2.27	0.62
2:L:59:GLN:CG	2:L:132:ARG:HB2	2.29	0.62
2:J:67:VAL:HG13	2:J:109:LEU:HD13	1.80	0.62
2:L:184:THR:HA	2:L:249:SER:HA	1.81	0.62
1:K:79:ARG:HB3	1:K:170:MET:HE1	1.80	0.62
2:B:172:LEU:HD23	2:B:172:LEU:O	2.00	0.62
1:A:135:ARG:HH22	1:A:181:ALA:CB	2.13	0.62
2:J:21:TYR:HB3	2:J:151:ASN:ND2	2.15	0.61
1:K:4:LEU:HD21	1:K:87:VAL:HG21	1.81	0.61
1:C:135:ARG:HH22	1:C:181:ALA:CB	2.13	0.61
2:F:59:GLN:CG	2:F:132:ARG:HD2	2.30	0.61
1:E:104:GLN:HG3	2:F:168:VAL:HG23	1.82	0.61
2:J:201:THR:CG2	2:J:206:ASN:HA	2.24	0.61
2:H:172:LEU:O	2:H:172:LEU:HD23	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:ARG:HH22	1:E:181:ALA:CB	2.14	0.61
2:F:172:LEU:HD23	2:F:172:LEU:O	2.01	0.61
1:G:135:ARG:HH22	1:G:181:ALA:CB	2.13	0.61
1:I:162:LEU:HD21	1:I:178:PRO:CD	2.29	0.61
2:J:19:ASN:HD21	2:L:219:GLN:HE22	1.48	0.61
1:M:79:ARG:HB3	1:M:170:MET:HE1	1.82	0.61
2:L:32:GLN:O	2:L:110:THR:HG23	1.99	0.61
1:E:185:ILE:HB	1:E:202:GLY:HA3	1.82	0.61
1:E:191:ASN:HD21	1:E:195:ALA:HB3	1.63	0.61
2:L:74:THR:HG22	2:L:83:PRO:HA	1.83	0.61
2:H:67:VAL:HG23	2:H:126:ILE:HG12	1.83	0.61
2:B:67:VAL:HG23	2:B:126:ILE:HG12	1.82	0.61
2:H:59:GLN:CG	2:H:132:ARG:HD2	2.30	0.61
1:E:140:LEU:HD23	1:E:141:THR:N	2.15	0.61
2:N:19:ASN:HD21	2:P:219:GLN:HE22	1.46	0.61
2:J:184:THR:HA	2:J:249:SER:HA	1.81	0.61
1:I:7:THR:O	1:I:111:ILE:HB	2.01	0.61
1:G:11:TYR:HB2	1:G:113:LEU:HD11	1.81	0.61
2:F:170:VAL:CG1	2:F:172:LEU:HB2	2.26	0.61
1:A:104:GLN:HG3	2:B:168:VAL:HG23	1.82	0.61
2:L:20:VAL:HG21	2:L:42:ILE:HD11	1.82	0.61
1:I:4:LEU:O	2:J:160:GLY:N	2.33	0.61
2:P:175:TYR:OH	2:P:263:VAL:HB	2.00	0.61
1:C:177:LEU:HD12	1:C:178:PRO:HD2	1.83	0.61
2:N:21:TYR:HB3	2:N:151:ASN:ND2	2.15	0.61
1:A:188:ARG:NH1	1:A:199:LYS:HB2	2.16	0.61
2:P:184:THR:HA	2:P:249:SER:HA	1.81	0.61
2:N:175:TYR:N	2:N:176:PRO:HD2	2.16	0.61
1:C:102:THR:HA	2:D:171:THR:HG22	1.82	0.60
2:H:174:ASP:O	2:H:176:PRO:N	2.34	0.60
2:P:20:VAL:HG21	2:P:42:ILE:HD11	1.81	0.60
2:H:92:ARG:HG3	2:H:92:ARG:NH1	2.11	0.60
2:N:193:LEU:HB3	2:N:240:LEU:HD12	1.83	0.60
2:D:175:TYR:O	2:D:256:TYR:CD1	2.54	0.60
1:O:27:GLU:CG	1:O:60:LYS:HD2	2.29	0.60
1:M:7:THR:O	1:M:111:ILE:HB	2.01	0.60
2:L:193:LEU:HB3	2:L:240:LEU:HD12	1.82	0.60
1:E:188:ARG:NH1	1:E:199:LYS:HB2	2.17	0.60
1:C:118:ALA:O	1:C:119:LYS:HB2	2.02	0.60
2:D:207:SER:O	2:D:224:GLN:HG3	2.02	0.60
2:D:170:VAL:CG1	2:D:172:LEU:HB2	2.26	0.60
1:E:102:THR:HA	2:F:171:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:20:VAL:HG21	2:N:42:ILE:HD11	1.82	0.60
1:K:7:THR:O	1:K:111:ILE:HB	2.00	0.60
2:J:74:THR:HG22	2:J:83:PRO:HA	1.82	0.60
2:H:192:ASN:ND2	2:H:279:GLN:HE22	1.96	0.60
2:P:21:TYR:HB3	2:P:151:ASN:ND2	2.15	0.60
2:L:14:GLY:HA2	2:L:142:PHE:CE1	2.37	0.60
2:P:74:THR:HG22	2:P:83:PRO:HA	1.82	0.60
1:A:11:TYR:HB2	1:A:113:LEU:HD11	1.83	0.60
2:J:175:TYR:OH	2:J:263:VAL:HB	2.01	0.60
2:L:125:LEU:HD12	2:L:148:ILE:O	2.02	0.60
2:J:175:TYR:N	2:J:176:PRO:HD2	2.16	0.60
2:L:201:THR:CG2	2:L:206:ASN:HA	2.24	0.60
1:A:177:LEU:HD12	1:A:178:PRO:HD2	1.83	0.60
1:C:104:GLN:HG3	2:D:168:VAL:HG23	1.84	0.60
1:O:117:PRO:O	1:O:120:LEU:HG	2.02	0.60
1:A:191:ASN:HD21	1:A:195:ALA:HB3	1.66	0.60
2:L:175:TYR:N	2:L:176:PRO:HD2	2.16	0.60
2:F:227:ARG:HB3	2:F:232:ILE:HD11	1.84	0.60
2:B:175:TYR:O	2:B:256:TYR:CD1	2.55	0.60
1:G:141:THR:HG23	1:G:174:THR:HG22	1.83	0.60
2:B:167:ASP:OD2	2:B:168:VAL:N	2.35	0.60
2:J:193:LEU:HB3	2:J:240:LEU:HD12	1.83	0.60
2:B:184:THR:HG22	2:B:249:SER:HA	1.82	0.60
2:B:174:ASP:O	2:B:176:PRO:N	2.35	0.60
2:F:174:ASP:O	2:F:176:PRO:N	2.35	0.60
1:E:177:LEU:HD12	1:E:178:PRO:HD2	1.83	0.60
1:E:94:ASP:HB3	1:E:96:SER:OG	2.01	0.60
2:P:175:TYR:N	2:P:176:PRO:HD2	2.16	0.60
2:L:175:TYR:OH	2:L:263:VAL:HB	2.01	0.60
2:L:21:TYR:HB3	2:L:151:ASN:ND2	2.16	0.59
1:K:4:LEU:O	2:L:160:GLY:N	2.33	0.59
2:N:175:TYR:OH	2:N:263:VAL:HB	2.00	0.59
2:P:193:LEU:HB3	2:P:240:LEU:HD12	1.82	0.59
2:N:74:THR:HG22	2:N:83:PRO:HA	1.82	0.59
2:P:125:LEU:HD12	2:P:148:ILE:O	2.02	0.59
1:I:101:ASN:ND2	2:J:268:VAL:HG23	2.17	0.59
2:F:184:THR:HG22	2:F:249:SER:HA	1.83	0.59
1:G:82:LEU:HD12	1:G:83:PHE:N	2.16	0.59
1:M:117:PRO:O	1:M:120:LEU:HG	2.02	0.59
1:A:102:THR:HA	2:B:171:THR:HG22	1.82	0.59
2:H:175:TYR:O	2:H:256:TYR:CD1	2.55	0.59
1:I:27:GLU:CG	1:I:60:LYS:HD2	2.29	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:82:LEU:HD12	1:C:83:PHE:N	2.17	0.59
2:H:163:VAL:HG22	2:H:185:VAL:HG12	1.84	0.59
2:H:167:ASP:OD2	2:H:168:VAL:N	2.36	0.59
1:K:101:ASN:ND2	2:L:268:VAL:HG23	2.17	0.59
2:L:177:GLY:HA3	2:L:256:TYR:CE1	2.38	0.59
1:I:117:PRO:O	1:I:120:LEU:HG	2.02	0.59
1:M:188:ARG:HH11	1:M:199:LYS:HB2	1.67	0.59
1:E:118:ALA:O	1:E:119:LYS:HB2	2.02	0.59
2:J:14:GLY:HA2	2:J:142:PHE:CE1	2.38	0.59
2:D:67:VAL:HG23	2:D:126:ILE:HG12	1.85	0.59
2:D:174:ASP:O	2:D:176:PRO:N	2.35	0.59
1:G:102:THR:HA	2:H:171:THR:HG22	1.82	0.59
1:G:188:ARG:NH1	1:G:199:LYS:HB2	2.17	0.59
1:K:117:PRO:O	1:K:120:LEU:HG	2.02	0.59
1:E:11:TYR:HB2	1:E:113:LEU:HD11	1.83	0.59
1:G:177:LEU:HD12	1:G:178:PRO:HD2	1.84	0.59
1:A:135:ARG:HH22	1:A:181:ALA:HB1	1.68	0.59
1:O:7:THR:O	1:O:111:ILE:HB	2.01	0.59
1:K:11:TYR:HB2	1:K:113:LEU:HD11	1.85	0.59
1:M:11:TYR:HB2	1:M:113:LEU:HD11	1.85	0.59
1:G:141:THR:CG2	1:G:174:THR:HG22	2.33	0.59
2:N:14:GLY:HA2	2:N:142:PHE:CE1	2.37	0.59
2:P:177:GLY:HA3	2:P:256:TYR:CE1	2.38	0.59
2:D:184:THR:HG22	2:D:249:SER:HA	1.85	0.59
2:H:227:ARG:HB3	2:H:232:ILE:HD11	1.85	0.59
1:O:156:ASN:C	1:O:158:GLY:H	2.06	0.59
2:F:175:TYR:O	2:F:256:TYR:CD1	2.55	0.59
1:M:4:LEU:O	2:N:160:GLY:N	2.33	0.59
2:F:13:ILE:HG13	4:F:1539:HOH:O	2.03	0.59
2:H:184:THR:HG22	2:H:249:SER:HA	1.84	0.59
1:I:156:ASN:C	1:I:158:GLY:H	2.07	0.59
1:G:118:ALA:O	1:G:119:LYS:HB2	2.02	0.59
1:A:82:LEU:HD12	1:A:83:PHE:N	2.18	0.59
1:C:179:SER:C	1:C:181:ALA:N	2.51	0.59
2:N:24:LEU:HD11	2:N:126:ILE:HD11	1.84	0.59
2:F:167:ASP:OD2	2:F:168:VAL:N	2.36	0.59
1:C:191:ASN:HD21	1:C:195:ALA:HB3	1.67	0.59
1:E:82:LEU:HD12	1:E:83:PHE:N	2.17	0.59
1:K:27:GLU:HG2	1:K:60:LYS:CD	2.32	0.58
2:N:177:GLY:HA3	2:N:256:TYR:CE1	2.37	0.58
2:P:14:GLY:HA2	2:P:142:PHE:CE1	2.37	0.58
1:I:188:ARG:HH11	1:I:199:LYS:HB2	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:188:ARG:NH1	1:C:199:LYS:HB2	2.17	0.58
1:G:27:GLU:HA	1:G:60:LYS:HG3	1.85	0.58
1:O:79:ARG:HA	1:O:147:PRO:HB2	1.85	0.58
1:G:47:ARG:HH22	1:G:74:GLN:HB2	1.69	0.58
1:K:27:GLU:CG	1:K:60:LYS:HD2	2.30	0.58
1:C:27:GLU:HA	1:C:60:LYS:HG3	1.85	0.58
1:I:103:LEU:O	2:J:168:VAL:HG23	2.03	0.58
2:F:5:THR:HG22	2:F:8:GLY:H	1.67	0.58
1:A:118:ALA:O	1:A:119:LYS:HB2	2.01	0.58
1:A:138:ASN:C	1:A:177:LEU:HB3	2.24	0.58
2:J:24:LEU:HD11	2:J:126:ILE:HD11	1.85	0.58
2:D:59:GLN:CG	2:D:132:ARG:HD2	2.31	0.58
1:K:188:ARG:HH11	1:K:199:LYS:HB2	1.68	0.58
2:B:227:ARG:HB3	2:B:232:ILE:HD11	1.86	0.58
2:H:114:SER:HB3	2:L:80:SER:HB3	1.85	0.58
2:N:125:LEU:HD12	2:N:148:ILE:O	2.02	0.58
2:P:24:LEU:HD11	2:P:126:ILE:HD11	1.85	0.58
1:I:135:ARG:NH1	1:I:181:ALA:CB	2.53	0.58
1:M:103:LEU:O	2:N:168:VAL:HG23	2.04	0.58
1:I:11:TYR:HB2	1:I:113:LEU:HD11	1.85	0.58
2:B:179:VAL:O	2:B:253:THR:HG23	2.03	0.58
1:M:101:ASN:ND2	2:N:268:VAL:HG23	2.17	0.58
2:B:58:LEU:H	2:B:90:THR:CG2	2.16	0.58
1:C:188:ARG:HH12	1:C:199:LYS:H	1.50	0.58
1:G:135:ARG:NH2	1:G:181:ALA:HB1	2.19	0.58
2:F:92:ARG:HG3	2:F:92:ARG:NH1	2.12	0.58
1:G:188:ARG:HH12	1:G:199:LYS:H	1.51	0.58
1:O:103:LEU:O	2:P:168:VAL:HG23	2.04	0.58
2:N:84:PHE:CD1	2:N:85:PRO:HA	2.39	0.58
1:I:197:THR:HB	1:I:198:PRO:HD2	1.86	0.58
2:N:131:LEU:HB3	2:N:144:PHE:HB2	1.86	0.58
1:O:11:TYR:HB2	1:O:113:LEU:HD11	1.85	0.58
2:N:201:THR:CG2	2:N:206:ASN:HA	2.24	0.58
2:H:170:VAL:CG1	2:H:172:LEU:HB2	2.27	0.58
1:G:135:ARG:HH22	1:G:181:ALA:HB1	1.68	0.58
2:F:192:ASN:ND2	2:F:279:GLN:HE22	1.99	0.58
2:H:58:LEU:H	2:H:90:THR:CG2	2.16	0.58
1:C:135:ARG:HH22	1:C:181:ALA:HB1	1.68	0.58
1:E:135:ARG:NH2	1:E:181:ALA:HB1	2.19	0.58
1:K:122:LEU:HD11	1:K:126:GLN:O	2.04	0.58
1:O:122:LEU:HD11	1:O:126:GLN:O	2.04	0.58
1:G:1:GLY:H1	1:G:26:ASP:CG	2.07	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:223:VAL:HG12	2:L:224:GLN:N	2.19	0.58
1:M:27:GLU:HG2	1:M:60:LYS:CD	2.32	0.58
1:M:79:ARG:HA	1:M:147:PRO:HB2	1.85	0.58
2:P:201:THR:CG2	2:P:206:ASN:HA	2.24	0.57
2:B:167:ASP:CG	2:B:168:VAL:N	2.50	0.57
1:E:138:ASN:C	1:E:177:LEU:HB3	2.24	0.57
2:D:167:ASP:OD2	2:D:168:VAL:N	2.35	0.57
1:A:27:GLU:HA	1:A:60:LYS:HG3	1.86	0.57
2:F:58:LEU:H	2:F:90:THR:CG2	2.16	0.57
1:O:4:LEU:O	2:P:160:GLY:N	2.33	0.57
1:K:6:ALA:HB3	1:K:20:LEU:HD11	1.86	0.57
2:B:68:LEU:O	2:P:87:THR:HG21	2.03	0.57
2:J:177:GLY:HA3	2:J:256:TYR:CE1	2.38	0.57
2:H:68:LEU:O	2:L:87:THR:HG21	2.04	0.57
1:O:197:THR:HB	1:O:198:PRO:HD2	1.86	0.57
1:G:135:ARG:CZ	1:G:181:ALA:HB1	2.34	0.57
1:I:27:GLU:HG2	1:I:60:LYS:CD	2.32	0.57
1:G:158:GLY:HA2	1:G:184:ASN:HD22	1.69	0.57
1:K:79:ARG:HA	1:K:147:PRO:HB2	1.85	0.57
1:A:24:ASN:O	1:A:60:LYS:HA	2.05	0.57
1:E:27:GLU:HA	1:E:60:LYS:HG3	1.87	0.57
1:I:122:LEU:HD11	1:I:126:GLN:O	2.04	0.57
1:O:6:ALA:HB3	1:O:20:LEU:HD11	1.86	0.57
1:C:138:ASN:C	1:C:177:LEU:HB3	2.24	0.57
1:O:101:ASN:ND2	2:P:268:VAL:HG23	2.17	0.57
1:O:188:ARG:HH11	1:O:199:LYS:HB2	1.68	0.57
2:L:131:LEU:HB3	2:L:144:PHE:HB2	1.87	0.57
1:C:135:ARG:NH2	1:C:181:ALA:HB1	2.19	0.57
2:B:120:ILE:CG2	2:B:126:ILE:HD11	2.31	0.57
2:L:84:PHE:CD1	2:L:85:PRO:HA	2.40	0.57
2:P:84:PHE:CD1	2:P:85:PRO:HA	2.39	0.57
1:C:134:ARG:CD	1:C:141:THR:CG2	2.83	0.57
1:G:138:ASN:C	1:G:177:LEU:HB3	2.25	0.57
2:J:125:LEU:HD12	2:J:148:ILE:O	2.03	0.57
1:M:156:ASN:C	1:M:158:GLY:H	2.06	0.57
2:D:5:THR:HG22	2:D:8:GLY:H	1.69	0.57
1:K:156:ASN:C	1:K:158:GLY:H	2.07	0.57
1:C:158:GLY:HA2	1:C:184:ASN:HD22	1.69	0.57
1:C:135:ARG:CZ	1:C:181:ALA:HB1	2.34	0.57
2:F:179:VAL:O	2:F:253:THR:HG23	2.03	0.57
2:L:24:LEU:HD11	2:L:126:ILE:HD11	1.84	0.57
1:A:135:ARG:NH2	1:A:181:ALA:HB1	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:103:LEU:O	2:L:168:VAL:HG23	2.04	0.57
2:L:71:PHE:CE2	2:L:111:PRO:HG3	2.39	0.57
2:N:71:PHE:CE2	2:N:111:PRO:HG3	2.39	0.57
1:E:197:THR:HB	1:E:198:PRO:HD2	1.87	0.57
2:B:114:SER:HB3	2:P:80:SER:HB3	1.85	0.57
1:I:79:ARG:HA	1:I:147:PRO:HB2	1.85	0.57
2:J:71:PHE:CE2	2:J:111:PRO:HG3	2.40	0.57
2:F:163:VAL:HG22	2:F:185:VAL:HG12	1.86	0.57
2:L:96:ASN:HD22	2:L:96:ASN:H	1.53	0.57
2:N:66:GLY:O	2:N:70:ASN:HB2	2.05	0.57
1:M:6:ALA:HB3	1:M:20:LEU:HD11	1.87	0.57
1:M:197:THR:HB	1:M:198:PRO:HD2	1.86	0.57
2:J:131:LEU:HB3	2:J:144:PHE:HB2	1.87	0.57
2:D:163:VAL:HG22	2:D:185:VAL:HG12	1.87	0.57
1:C:134:ARG:NH1	1:C:141:THR:HG21	2.19	0.57
2:D:58:LEU:H	2:D:90:THR:CG2	2.18	0.57
2:P:71:PHE:CE2	2:P:111:PRO:HG3	2.40	0.57
2:P:131:LEU:HB3	2:P:144:PHE:HB2	1.87	0.57
2:P:227:ARG:HH22	2:P:230:THR:HG21	1.70	0.57
2:J:223:VAL:HG12	2:J:224:GLN:N	2.19	0.57
2:N:224:GLN:HG2	2:N:231:ILE:CG2	2.35	0.57
2:L:227:ARG:HH22	2:L:230:THR:HG21	1.70	0.57
2:L:267:ASN:HB3	2:L:269:GLN:HG3	1.87	0.57
1:M:28:ASN:HD22	1:M:28:ASN:N	2.03	0.57
2:B:5:THR:HG22	2:B:8:GLY:H	1.69	0.57
1:C:188:ARG:NH1	1:C:199:LYS:N	2.53	0.57
2:H:5:THR:HG22	2:H:8:GLY:H	1.70	0.57
1:A:135:ARG:CZ	1:A:181:ALA:HB1	2.34	0.57
1:E:135:ARG:HH22	1:E:181:ALA:HB1	1.68	0.57
1:M:122:LEU:HD11	1:M:126:GLN:O	2.04	0.57
2:J:84:PHE:CD1	2:J:85:PRO:HA	2.40	0.57
2:P:224:GLN:HG2	2:P:231:ILE:CG2	2.35	0.56
1:E:135:ARG:CZ	1:E:181:ALA:HB1	2.34	0.56
1:E:158:GLY:HA2	1:E:184:ASN:HD22	1.69	0.56
1:O:11:TYR:CE2	1:O:69:ASP:HB2	2.40	0.56
1:K:197:THR:HB	1:K:198:PRO:HD2	1.86	0.56
2:J:96:ASN:H	2:J:96:ASN:HD22	1.53	0.56
2:D:136:ASN:C	2:D:136:ASN:HD22	2.08	0.56
1:K:28:ASN:N	1:K:28:ASN:HD22	2.03	0.56
2:D:179:VAL:O	2:D:253:THR:HG23	2.05	0.56
1:A:158:GLY:HA2	1:A:184:ASN:HD22	1.69	0.56
2:L:11:ILE:HD12	2:L:146:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:24:ASN:O	1:E:60:LYS:HA	2.05	0.56
2:B:219:GLN:HG2	2:B:220:GLY:N	2.20	0.56
2:H:219:GLN:HG2	2:H:220:GLY:N	2.20	0.56
2:D:219:GLN:HG2	2:D:220:GLY:N	2.19	0.56
2:P:267:ASN:HB3	2:P:269:GLN:HG3	1.87	0.56
1:G:193:TYR:O	2:H:158:THR:HG22	2.06	0.56
1:M:11:TYR:CE2	1:M:69:ASP:HB2	2.40	0.56
2:J:66:GLY:O	2:J:70:ASN:HB2	2.05	0.56
2:H:28:VAL:O	2:H:156:VAL:HA	2.06	0.56
2:J:250:LEU:HB2	2:J:252:LEU:HG	1.87	0.56
1:E:193:TYR:O	2:F:158:THR:HG22	2.06	0.56
2:N:227:ARG:HH22	2:N:230:THR:HG21	1.70	0.56
2:F:226:THR:HG22	2:F:253:THR:HB	1.88	0.56
2:H:179:VAL:O	2:H:253:THR:HG23	2.05	0.56
1:A:188:ARG:NH1	1:A:199:LYS:N	2.53	0.56
2:N:11:ILE:HD12	2:N:146:TRP:CZ2	2.40	0.56
1:I:11:TYR:CE2	1:I:69:ASP:HB2	2.40	0.56
1:O:154:GLU:OE2	1:O:188:ARG:HD3	2.06	0.56
2:H:120:ILE:HD13	2:H:126:ILE:HD11	1.87	0.56
2:N:224:GLN:HG2	2:N:231:ILE:HG21	1.87	0.56
2:P:264:THR:CG2	2:P:265:ALA:H	2.15	0.56
1:G:188:ARG:NH1	1:G:199:LYS:N	2.54	0.56
2:J:30:VAL:HA	2:J:111:PRO:HB2	1.87	0.56
2:D:227:ARG:HB3	2:D:232:ILE:HD11	1.88	0.56
2:P:223:VAL:HG12	2:P:224:GLN:N	2.19	0.56
1:C:47:ARG:HH22	1:C:74:GLN:HB2	1.70	0.56
1:E:188:ARG:HH12	1:E:199:LYS:H	1.52	0.56
1:K:189:THR:O	1:K:196:LEU:HA	2.06	0.56
2:J:227:ARG:HH22	2:J:230:THR:HG21	1.70	0.56
1:O:189:THR:O	1:O:196:LEU:HA	2.06	0.56
1:I:6:ALA:HB3	1:I:20:LEU:HD11	1.86	0.56
2:J:224:GLN:HG2	2:J:231:ILE:CG2	2.35	0.56
2:L:224:GLN:HG2	2:L:231:ILE:CG2	2.35	0.56
1:I:162:LEU:CD2	1:I:178:PRO:HD3	2.36	0.56
1:I:135:ARG:HH12	1:I:181:ALA:HB2	1.69	0.56
1:K:80:GLU:HG3	1:K:147:PRO:O	2.05	0.56
2:N:267:ASN:HB3	2:N:269:GLN:HG3	1.87	0.56
1:C:193:TYR:O	2:D:158:THR:HG22	2.06	0.56
2:B:163:VAL:HG22	2:B:185:VAL:HG12	1.88	0.56
1:G:197:THR:HB	1:G:198:PRO:HD2	1.88	0.56
1:O:27:GLU:HG2	1:O:60:LYS:CD	2.32	0.56
2:J:11:ILE:HD12	2:J:146:TRP:CZ2	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:80:GLU:HG3	1:O:147:PRO:O	2.06	0.56
2:P:60:ARG:HG3	2:P:61:GLY:N	2.21	0.56
2:P:66:GLY:O	2:P:70:ASN:HB2	2.06	0.56
2:B:28:VAL:O	2:B:156:VAL:HA	2.05	0.56
1:M:22:VAL:CG2	1:M:65:LEU:HG	2.36	0.56
1:E:142:LEU:CD2	1:E:142:LEU:H	2.19	0.56
2:P:224:GLN:HG2	2:P:231:ILE:HG21	1.88	0.56
2:N:223:VAL:HG12	2:N:224:GLN:N	2.20	0.56
1:E:188:ARG:NH1	1:E:199:LYS:N	2.54	0.56
1:K:11:TYR:CE2	1:K:69:ASP:HB2	2.40	0.56
2:B:226:THR:HG22	2:B:253:THR:HB	1.88	0.56
1:A:188:ARG:HH12	1:A:199:LYS:H	1.51	0.56
2:F:219:GLN:HG2	2:F:220:GLY:N	2.20	0.56
2:L:60:ARG:HG3	2:L:61:GLY:N	2.21	0.56
2:F:28:VAL:O	2:F:156:VAL:HA	2.05	0.56
1:E:47:ARG:HH22	1:E:74:GLN:HB2	1.69	0.55
1:G:141:THR:CB	1:G:174:THR:HG22	2.35	0.55
1:K:162:LEU:CD2	1:K:178:PRO:HD3	2.36	0.55
2:L:20:VAL:HG12	2:L:22:VAL:HG13	1.88	0.55
1:M:80:GLU:HG3	1:M:147:PRO:O	2.06	0.55
2:J:267:ASN:HB3	2:J:269:GLN:HG3	1.87	0.55
2:P:30:VAL:HA	2:P:111:PRO:HB2	1.89	0.55
2:D:28:VAL:O	2:D:156:VAL:HA	2.07	0.55
1:K:22:VAL:CG2	1:K:65:LEU:HG	2.36	0.55
2:P:250:LEU:HB2	2:P:252:LEU:HG	1.87	0.55
1:A:197:THR:HB	1:A:198:PRO:HD2	1.88	0.55
2:H:207:SER:O	2:H:224:GLN:HG3	2.06	0.55
1:A:47:ARG:HH22	1:A:74:GLN:HB2	1.71	0.55
2:N:264:THR:CG2	2:N:265:ALA:H	2.16	0.55
1:I:154:GLU:OE2	1:I:188:ARG:HD3	2.06	0.55
2:F:71:PHE:CE2	2:F:111:PRO:HG3	2.41	0.55
2:D:120:ILE:HD13	2:D:126:ILE:HD11	1.87	0.55
2:H:226:THR:HG22	2:H:253:THR:HB	1.88	0.55
2:N:220:GLY:HA2	2:N:259:THR:OG1	2.07	0.55
2:P:220:GLY:HA2	2:P:259:THR:OG1	2.07	0.55
2:P:96:ASN:H	2:P:96:ASN:HD22	1.54	0.55
1:O:22:VAL:CG2	1:O:65:LEU:HG	2.36	0.55
1:I:22:VAL:CG2	1:I:65:LEU:HG	2.37	0.55
2:B:207:SER:O	2:B:224:GLN:HG3	2.06	0.55
1:O:28:ASN:N	1:O:28:ASN:HD22	2.03	0.55
2:F:131:LEU:C	2:F:131:LEU:HD23	2.27	0.55
2:B:201:THR:CG2	2:B:206:ASN:HA	2.29	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:201:THR:CG2	2:F:206:ASN:HD22	2.18	0.55
2:N:20:VAL:HG12	2:N:22:VAL:HG13	1.89	0.55
2:P:11:ILE:HD12	2:P:146:TRP:CZ2	2.40	0.55
1:I:104:GLN:O	2:J:271:ILE:HA	2.07	0.55
2:L:66:GLY:O	2:L:70:ASN:HB2	2.05	0.55
2:F:83:PRO:O	2:F:86:THR:HA	2.07	0.55
1:G:142:LEU:CD2	1:G:142:LEU:H	2.19	0.55
1:A:142:LEU:H	1:A:142:LEU:CD2	2.20	0.55
1:M:162:LEU:CD2	1:M:178:PRO:HD3	2.36	0.55
2:N:19:ASN:ND2	2:P:219:GLN:NE2	2.53	0.55
2:P:117:GLY:O	2:P:155:VAL:HA	2.06	0.55
2:L:30:VAL:HA	2:L:111:PRO:HB2	1.87	0.55
1:M:104:GLN:O	2:N:271:ILE:HA	2.07	0.55
1:I:28:ASN:N	1:I:28:ASN:HD22	2.03	0.55
2:B:136:ASN:C	2:B:136:ASN:HD22	2.09	0.55
2:J:28:VAL:O	2:J:156:VAL:HA	2.07	0.55
2:H:131:LEU:HD23	2:H:131:LEU:C	2.27	0.55
2:F:120:ILE:CG2	2:F:126:ILE:HD11	2.29	0.55
1:O:135:ARG:HH12	1:O:181:ALA:HB2	1.68	0.55
1:I:80:GLU:HG3	1:I:147:PRO:O	2.06	0.55
1:M:154:GLU:OE2	1:M:188:ARG:HD3	2.06	0.55
1:M:184:ASN:O	1:M:186:THR:HG23	2.07	0.55
1:I:28:ASN:N	1:I:28:ASN:ND2	2.54	0.55
2:J:73:GLY:HA2	4:J:1611:HOH:O	2.06	0.55
2:N:250:LEU:HB2	2:N:252:LEU:HG	1.88	0.55
1:I:189:THR:O	1:I:196:LEU:HA	2.07	0.55
2:J:19:ASN:ND2	2:L:219:GLN:NE2	2.54	0.55
2:J:117:GLY:O	2:J:155:VAL:HA	2.07	0.55
1:M:28:ASN:H	1:M:28:ASN:HD22	1.54	0.55
2:L:4:LYS:HA	2:L:10:ALA:HA	1.89	0.55
1:C:142:LEU:CD2	1:C:142:LEU:H	2.20	0.55
2:F:117:GLY:O	2:F:155:VAL:HA	2.07	0.55
2:H:201:THR:CG2	2:H:206:ASN:HD22	2.18	0.55
2:L:71:PHE:HE2	2:L:111:PRO:HG3	1.72	0.55
2:D:201:THR:CG2	2:D:206:ASN:HD22	2.18	0.55
1:E:140:LEU:HB2	1:E:177:LEU:HD22	1.89	0.55
1:M:28:ASN:N	1:M:28:ASN:ND2	2.54	0.55
2:L:250:LEU:HB2	2:L:252:LEU:HG	1.87	0.55
2:J:224:GLN:HG2	2:J:231:ILE:HG21	1.88	0.54
1:O:184:ASN:O	1:O:186:THR:HG23	2.08	0.54
1:K:28:ASN:HD22	1:K:28:ASN:H	1.54	0.54
2:H:71:PHE:CE2	2:H:111:PRO:HG3	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:THR:HG23	1:A:174:THR:O	2.06	0.54
2:F:136:ASN:C	2:F:136:ASN:HD22	2.09	0.54
1:M:115:TYR:O	1:M:117:PRO:HD3	2.08	0.54
2:J:4:LYS:HA	2:J:10:ALA:HA	1.89	0.54
2:L:200:THR:O	2:L:209:PHE:HA	2.07	0.54
2:P:200:THR:O	2:P:209:PHE:HA	2.07	0.54
2:P:28:VAL:O	2:P:156:VAL:HA	2.07	0.54
1:K:115:TYR:O	1:K:117:PRO:HD3	2.07	0.54
1:K:184:ASN:O	1:K:186:THR:HG23	2.07	0.54
1:K:28:ASN:N	1:K:28:ASN:ND2	2.54	0.54
1:M:189:THR:O	1:M:196:LEU:HA	2.06	0.54
2:D:131:LEU:C	2:D:131:LEU:HD23	2.28	0.54
2:F:120:ILE:HD13	2:F:126:ILE:HD11	1.89	0.54
2:J:200:THR:O	2:J:209:PHE:HA	2.07	0.54
2:F:170:VAL:C	2:F:172:LEU:H	2.10	0.54
2:L:162:ASP:O	2:L:185:VAL:HG13	2.07	0.54
1:C:24:ASN:O	1:C:60:LYS:HA	2.06	0.54
1:K:104:GLN:O	2:L:271:ILE:HA	2.07	0.54
2:L:224:GLN:HG2	2:L:231:ILE:HG21	1.88	0.54
2:J:162:ASP:O	2:J:185:VAL:HG13	2.07	0.54
2:H:117:GLY:O	2:H:155:VAL:HA	2.07	0.54
2:N:200:THR:O	2:N:209:PHE:HA	2.08	0.54
2:F:172:LEU:O	2:F:173:PRO:C	2.46	0.54
1:O:162:LEU:CD2	1:O:178:PRO:HD3	2.36	0.54
1:I:185:ILE:HD12	1:I:204:MET:SD	2.48	0.54
2:N:60:ARG:HG3	2:N:61:GLY:N	2.22	0.54
2:D:71:PHE:CE2	2:D:111:PRO:HG3	2.42	0.54
2:J:201:THR:HA	2:J:209:PHE:HA	1.90	0.54
2:J:264:THR:CG2	2:J:265:ALA:H	2.16	0.54
2:L:264:THR:CG2	2:L:265:ALA:H	2.15	0.54
1:K:135:ARG:HH12	1:K:181:ALA:HB2	1.69	0.54
2:J:20:VAL:HG12	2:J:22:VAL:HG13	1.88	0.54
1:G:24:ASN:O	1:G:60:LYS:HA	2.07	0.54
2:L:74:THR:HB	2:L:82:TYR:O	2.07	0.54
1:I:115:TYR:O	1:I:117:PRO:HD3	2.07	0.54
2:F:5:THR:HG23	2:F:7:ASN:H	1.72	0.54
1:O:28:ASN:HD22	1:O:28:ASN:H	1.55	0.54
2:N:96:ASN:H	2:N:96:ASN:HD22	1.55	0.54
2:P:162:ASP:O	2:P:185:VAL:HG13	2.07	0.54
2:N:117:GLY:O	2:N:155:VAL:HA	2.07	0.54
1:K:154:GLU:OE2	1:K:188:ARG:HD3	2.06	0.54
1:I:28:ASN:H	1:I:28:ASN:HD22	1.54	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:201:THR:HA	2:L:209:PHE:HA	1.90	0.54
1:K:185:ILE:HD12	1:K:204:MET:SD	2.48	0.54
2:H:136:ASN:C	2:H:136:ASN:HD22	2.09	0.54
2:J:220:GLY:HA2	2:J:259:THR:OG1	2.07	0.54
2:N:28:VAL:O	2:N:156:VAL:HA	2.07	0.54
2:L:40:THR:O	2:L:40:THR:HG22	2.08	0.54
2:N:74:THR:HB	2:N:82:TYR:O	2.07	0.54
1:O:28:ASN:N	1:O:28:ASN:ND2	2.54	0.54
1:I:131:LEU:HD12	1:I:143:ILE:O	2.08	0.54
2:D:83:PRO:O	2:D:86:THR:HA	2.07	0.54
2:B:201:THR:CG2	2:B:206:ASN:HD22	2.20	0.54
2:H:201:THR:CG2	2:H:206:ASN:HA	2.29	0.54
1:E:183:SER:C	1:E:185:ILE:H	2.12	0.54
1:O:133:PHE:CE1	1:O:202:GLY:HA2	2.43	0.54
1:G:186:THR:HG21	1:G:199:LYS:HZ1	1.73	0.54
1:O:104:GLN:O	2:P:271:ILE:HA	2.07	0.54
1:O:115:TYR:O	1:O:117:PRO:HD3	2.08	0.54
2:F:207:SER:O	2:F:224:GLN:HG3	2.08	0.54
1:C:134:ARG:HD2	1:C:141:THR:HG22	1.91	0.53
1:G:140:LEU:HB2	1:G:177:LEU:HD22	1.90	0.53
1:G:133:PHE:CD2	1:G:140:LEU:HD21	2.31	0.53
1:M:185:ILE:HD12	1:M:204:MET:SD	2.48	0.53
2:P:71:PHE:HE2	2:P:111:PRO:HG3	1.74	0.53
1:A:193:TYR:O	2:B:158:THR:HG22	2.06	0.53
2:P:192:ASN:HB2	2:P:279:GLN:NE2	2.23	0.53
1:K:131:LEU:HD12	1:K:143:ILE:O	2.08	0.53
2:N:162:ASP:O	2:N:185:VAL:HG13	2.07	0.53
1:A:183:SER:C	1:A:185:ILE:H	2.12	0.53
1:O:185:ILE:HD12	1:O:204:MET:SD	2.48	0.53
1:G:183:SER:C	1:G:185:ILE:H	2.12	0.53
2:B:71:PHE:CE2	2:B:111:PRO:HG3	2.43	0.53
2:N:192:ASN:HB2	2:N:279:GLN:NE2	2.23	0.53
2:J:192:ASN:HB2	2:J:279:GLN:NE2	2.24	0.53
2:J:224:GLN:NE2	2:J:231:ILE:HD13	2.23	0.53
2:N:224:GLN:NE2	2:N:231:ILE:HD13	2.24	0.53
1:E:174:THR:O	1:E:174:THR:HG23	2.07	0.53
2:L:117:GLY:O	2:L:155:VAL:HA	2.08	0.53
2:N:30:VAL:HA	2:N:111:PRO:HB2	1.88	0.53
2:N:40:THR:HG22	2:N:40:THR:O	2.09	0.53
2:J:74:THR:HB	2:J:82:TYR:O	2.08	0.53
2:P:74:THR:HB	2:P:82:TYR:O	2.08	0.53
1:C:140:LEU:HB2	1:C:177:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:184:ASN:O	1:C:186:THR:HG23	2.09	0.53
2:P:224:GLN:NE2	2:P:231:ILE:HD13	2.24	0.53
2:D:120:ILE:CG2	2:D:126:ILE:HD11	2.30	0.53
2:H:5:THR:HG23	2:H:7:ASN:H	1.73	0.53
1:M:101:ASN:ND2	2:N:268:VAL:H	2.07	0.53
1:K:101:ASN:ND2	2:L:268:VAL:H	2.07	0.53
2:P:40:THR:O	2:P:40:THR:HG22	2.08	0.53
2:J:174:ASP:HB3	2:J:176:PRO:HD2	1.91	0.53
2:B:170:VAL:C	2:B:172:LEU:H	2.11	0.53
2:L:28:VAL:O	2:L:156:VAL:HA	2.08	0.53
2:B:131:LEU:HD23	2:B:131:LEU:C	2.29	0.53
1:C:205:GLU:OXT	1:C:205:GLU:HG3	2.09	0.53
2:H:172:LEU:O	2:H:173:PRO:C	2.46	0.53
1:G:205:GLU:OXT	1:G:205:GLU:HG3	2.09	0.53
1:A:140:LEU:HB2	1:A:177:LEU:HD22	1.91	0.53
2:J:60:ARG:HG3	2:J:61:GLY:N	2.23	0.53
2:H:173:PRO:HG3	2:H:179:VAL:CG1	2.39	0.53
1:K:133:PHE:CE1	1:K:202:GLY:HA2	2.44	0.53
1:I:133:PHE:CE1	1:I:202:GLY:HA2	2.43	0.53
2:P:20:VAL:HG12	2:P:22:VAL:HG13	1.89	0.53
2:N:71:PHE:HE2	2:N:111:PRO:HG3	1.73	0.53
2:H:83:PRO:O	2:H:86:THR:HA	2.08	0.53
2:P:4:LYS:HA	2:P:10:ALA:HA	1.90	0.53
1:C:186:THR:HG21	1:C:199:LYS:NZ	2.23	0.53
2:D:63:ALA:HB1	2:D:67:VAL:HG12	1.89	0.53
2:D:170:VAL:C	2:D:172:LEU:H	2.12	0.53
2:L:174:ASP:HB3	2:L:176:PRO:HD2	1.91	0.53
2:B:172:LEU:O	2:B:173:PRO:C	2.47	0.53
2:H:7:ASN:HB2	4:H:1661:HOH:O	2.09	0.53
2:D:211:ASN:C	2:D:211:ASN:HD22	2.12	0.53
2:L:220:GLY:HA2	2:L:259:THR:OG1	2.06	0.53
2:L:192:ASN:HB2	2:L:279:GLN:NE2	2.24	0.53
1:G:184:ASN:O	1:G:186:THR:HG23	2.08	0.53
1:I:101:ASN:ND2	2:J:268:VAL:H	2.07	0.53
1:C:197:THR:HB	1:C:198:PRO:HD2	1.90	0.53
1:M:191:ASN:HD21	1:M:195:ALA:HB3	1.74	0.53
2:N:201:THR:HA	2:N:209:PHE:HA	1.90	0.53
1:E:186:THR:HG21	1:E:199:LYS:NZ	2.24	0.53
1:M:133:PHE:CE1	1:M:202:GLY:HA2	2.44	0.53
2:P:34:LEU:HD12	2:P:35:VAL:N	2.20	0.53
2:P:174:ASP:HB3	2:P:176:PRO:HD2	1.91	0.53
2:N:4:LYS:HA	2:N:10:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:46:GLY:O	1:O:70:ALA:HB3	2.09	0.53
2:L:224:GLN:NE2	2:L:231:ILE:HD13	2.24	0.52
2:H:211:ASN:HD22	2:H:211:ASN:C	2.10	0.52
2:F:211:ASN:C	2:F:211:ASN:HD22	2.11	0.52
2:N:174:ASP:HB3	2:N:176:PRO:HD2	1.91	0.52
1:M:28:ASN:O	1:M:29:SER:HB3	2.09	0.52
2:L:78:SER:H	2:L:104:PRO:HB2	1.74	0.52
1:M:46:GLY:O	1:M:70:ALA:HB3	2.10	0.52
2:J:71:PHE:HE2	2:J:111:PRO:HG3	1.73	0.52
1:C:183:SER:C	1:C:185:ILE:H	2.12	0.52
2:P:207:SER:O	2:P:224:GLN:HG3	2.10	0.52
2:P:201:THR:HA	2:P:209:PHE:HA	1.90	0.52
2:H:167:ASP:CG	2:H:168:VAL:N	2.50	0.52
2:B:185:VAL:HG23	2:B:243:VAL:HG11	1.90	0.52
1:E:22:VAL:CG2	1:E:65:LEU:HG	2.39	0.52
2:J:78:SER:H	2:J:104:PRO:HB2	1.75	0.52
1:O:131:LEU:HD12	1:O:143:ILE:O	2.09	0.52
2:P:78:SER:H	2:P:104:PRO:HB2	1.75	0.52
2:B:120:ILE:HD13	2:B:126:ILE:HD11	1.90	0.52
2:L:208:ILE:HG21	2:L:259:THR:HG22	1.91	0.52
2:D:117:GLY:O	2:D:155:VAL:HA	2.08	0.52
1:A:184:ASN:O	1:A:186:THR:HG23	2.08	0.52
1:M:135:ARG:HH12	1:M:181:ALA:HB2	1.68	0.52
1:O:101:ASN:ND2	2:P:268:VAL:H	2.07	0.52
1:I:184:ASN:O	1:I:186:THR:HG23	2.08	0.52
1:I:46:GLY:O	1:I:70:ALA:HB3	2.09	0.52
2:D:22:VAL:HG23	2:D:22:VAL:O	2.09	0.52
2:B:174:ASP:O	2:B:176:PRO:CD	2.58	0.52
2:D:174:ASP:O	2:D:176:PRO:CD	2.58	0.52
1:E:184:ASN:O	1:E:186:THR:HG23	2.08	0.52
1:I:140:LEU:HD23	1:I:141:THR:N	2.25	0.52
2:N:208:ILE:HG21	2:N:259:THR:HG22	1.92	0.52
1:G:186:THR:HG21	1:G:199:LYS:NZ	2.23	0.52
1:C:122:LEU:CD1	1:C:126:GLN:HB3	2.40	0.52
2:H:185:VAL:HG23	2:H:243:VAL:HG11	1.92	0.52
1:K:28:ASN:O	1:K:29:SER:HB3	2.09	0.52
2:N:13:ILE:HG23	3:N:1506:MAN:C2	2.40	0.52
1:O:191:ASN:HD21	1:O:195:ALA:HB3	1.74	0.52
1:O:140:LEU:HD23	1:O:141:THR:N	2.25	0.52
2:N:14:GLY:HA2	2:N:142:PHE:CD1	2.45	0.52
1:M:131:LEU:HD12	1:M:143:ILE:O	2.08	0.52
2:B:83:PRO:O	2:B:86:THR:HA	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:174:ASP:O	2:H:176:PRO:CD	2.58	0.52
2:L:43:PHE:CD1	2:L:43:PHE:N	2.78	0.52
1:O:28:ASN:O	1:O:29:SER:HB3	2.09	0.52
1:K:191:ASN:HD21	1:K:195:ALA:HB3	1.74	0.52
1:K:46:GLY:O	1:K:70:ALA:HB3	2.09	0.52
2:B:211:ASN:C	2:B:211:ASN:HD22	2.12	0.52
1:K:140:LEU:HD23	1:K:141:THR:N	2.25	0.52
2:J:40:THR:O	2:J:40:THR:HG22	2.09	0.52
2:P:14:GLY:HA2	2:P:142:PHE:CD1	2.45	0.52
2:B:5:THR:HG23	2:B:7:ASN:H	1.73	0.52
1:C:186:THR:HG21	1:C:199:LYS:HZ1	1.75	0.51
2:B:173:PRO:HG3	2:B:179:VAL:CG1	2.39	0.51
1:E:205:GLU:HG3	1:E:205:GLU:OXT	2.09	0.51
2:N:164:SER:HB2	2:N:184:THR:O	2.10	0.51
1:M:79:ARG:HB3	1:M:170:MET:HE3	1.91	0.51
1:I:191:ASN:HD21	1:I:195:ALA:HB3	1.74	0.51
2:H:63:ALA:HB1	2:H:67:VAL:HG12	1.91	0.51
2:D:172:LEU:O	2:D:173:PRO:C	2.47	0.51
2:H:170:VAL:C	2:H:172:LEU:H	2.12	0.51
1:A:186:THR:HG21	1:A:199:LYS:NZ	2.25	0.51
1:O:160:ARG:CG	1:O:178:PRO:HG3	2.41	0.51
2:N:34:LEU:HD12	2:N:35:VAL:N	2.20	0.51
1:A:85:MET:O	1:A:110:ARG:HA	2.10	0.51
2:F:33:ASN:ND2	2:F:110:THR:OG1	2.44	0.51
1:C:144:ASN:OD1	1:C:146:THR:HG23	2.10	0.51
2:L:14:GLY:HA2	2:L:142:PHE:CD1	2.45	0.51
2:F:185:VAL:HG23	2:F:243:VAL:HG11	1.91	0.51
2:N:78:SER:H	2:N:104:PRO:HB2	1.75	0.51
1:A:133:PHE:CD2	1:A:140:LEU:HD21	2.30	0.51
1:M:160:ARG:CG	1:M:178:PRO:HG3	2.41	0.51
1:E:85:MET:O	1:E:110:ARG:HA	2.10	0.51
2:N:207:SER:O	2:N:224:GLN:HG3	2.10	0.51
2:H:211:ASN:ND2	2:H:269:GLN:H	2.09	0.51
2:P:208:ILE:HG21	2:P:259:THR:HG22	1.92	0.51
1:A:144:ASN:OD1	1:A:146:THR:HG23	2.10	0.51
1:G:144:ASN:OD1	1:G:146:THR:HG23	2.11	0.51
1:E:122:LEU:CD1	1:E:126:GLN:HB3	2.40	0.51
1:I:28:ASN:O	1:I:29:SER:HB3	2.09	0.51
1:E:1:GLY:H1	1:E:26:ASP:CG	2.14	0.51
2:F:50:GLU:H	2:F:50:GLU:CD	2.14	0.51
2:L:215:PHE:CD2	2:L:215:PHE:C	2.84	0.51
2:D:211:ASN:HD21	2:D:269:GLN:H	1.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:GLY:H1	1:A:26:ASP:CG	2.14	0.51
2:H:50:GLU:CD	2:H:50:GLU:H	2.14	0.51
2:F:211:ASN:HD21	2:F:269:GLN:H	1.57	0.51
1:K:160:ARG:CG	1:K:178:PRO:HG3	2.41	0.51
2:N:43:PHE:N	2:N:43:PHE:CD1	2.78	0.51
1:A:122:LEU:CD1	1:A:126:GLN:HB3	2.40	0.51
1:C:13:ALA:HB3	1:C:118:ALA:H	1.76	0.51
2:B:117:GLY:O	2:B:155:VAL:HA	2.09	0.51
2:H:120:ILE:CG2	2:H:126:ILE:HD11	2.31	0.51
2:J:67:VAL:HG21	2:J:126:ILE:CG2	2.35	0.51
2:J:208:ILE:HG21	2:J:259:THR:HG22	1.91	0.51
2:F:67:VAL:CG2	2:F:126:ILE:HG12	2.41	0.51
1:M:140:LEU:HD23	1:M:141:THR:N	2.25	0.51
2:P:190:SER:HA	2:P:244:GLY:HA2	1.93	0.51
2:J:43:PHE:N	2:J:43:PHE:CD1	2.79	0.51
1:A:22:VAL:CG2	1:A:65:LEU:HG	2.41	0.51
1:I:66:ARG:HH11	1:I:66:ARG:HG2	1.75	0.51
1:M:66:ARG:HH11	1:M:66:ARG:HG2	1.76	0.51
2:F:174:ASP:O	2:F:176:PRO:CD	2.59	0.51
2:H:211:ASN:HD21	2:H:269:GLN:H	1.57	0.51
2:P:43:PHE:CD1	2:P:43:PHE:N	2.78	0.51
2:D:5:THR:HG23	2:D:7:ASN:H	1.76	0.51
1:C:22:VAL:CG2	1:C:65:LEU:HG	2.41	0.51
1:K:66:ARG:HH11	1:K:66:ARG:HG2	1.76	0.51
2:D:174:ASP:O	2:D:176:PRO:HD2	2.11	0.51
2:H:174:ASP:O	2:H:176:PRO:HD2	2.11	0.51
1:A:205:GLU:HG3	1:A:205:GLU:OXT	2.10	0.51
1:I:160:ARG:CG	1:I:178:PRO:HG3	2.41	0.51
2:P:164:SER:HB2	2:P:184:THR:O	2.11	0.51
1:O:67:ILE:N	1:O:67:ILE:HD12	2.26	0.51
1:M:47:ARG:HH22	1:M:74:GLN:HB2	1.76	0.50
2:N:190:SER:HA	2:N:244:GLY:HA2	1.93	0.50
1:G:122:LEU:CD1	1:G:126:GLN:HB3	2.40	0.50
2:L:96:ASN:ND2	2:L:96:ASN:N	2.58	0.50
2:B:163:VAL:CG1	2:B:183:LEU:HD21	2.41	0.50
2:N:96:ASN:N	2:N:96:ASN:ND2	2.60	0.50
2:D:226:THR:HG22	2:D:253:THR:HB	1.94	0.50
2:L:163:VAL:HA	2:L:185:VAL:CG2	2.35	0.50
2:B:227:ARG:HA	2:B:251:GLY:O	2.11	0.50
1:I:9:VAL:O	1:I:113:LEU:HA	2.11	0.50
2:B:131:LEU:HB3	2:B:144:PHE:HB2	1.93	0.50
2:B:174:ASP:O	2:B:176:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:202:ALA:HB2	2:L:210:THR:CG2	2.34	0.50
1:E:133:PHE:CD2	1:E:140:LEU:HD21	2.31	0.50
2:H:33:ASN:ND2	2:H:110:THR:OG1	2.44	0.50
2:H:184:THR:HG22	2:H:249:SER:CA	2.41	0.50
1:A:13:ALA:HB3	1:A:118:ALA:H	1.76	0.50
2:J:96:ASN:N	2:J:96:ASN:ND2	2.59	0.50
2:P:96:ASN:ND2	2:P:96:ASN:N	2.59	0.50
2:J:215:PHE:C	2:J:215:PHE:CD2	2.84	0.50
2:J:207:SER:O	2:J:224:GLN:HG3	2.10	0.50
1:K:47:ARG:HH22	1:K:74:GLN:HB2	1.76	0.50
1:C:94:ASP:CG	2:D:168:VAL:HG11	2.32	0.50
1:E:144:ASN:OD1	1:E:146:THR:HG23	2.12	0.50
2:J:14:GLY:HA2	2:J:142:PHE:CD1	2.47	0.50
2:L:66:GLY:HA3	2:L:119:ALA:O	2.11	0.50
1:K:67:ILE:N	1:K:67:ILE:HD12	2.26	0.50
2:D:211:ASN:ND2	2:D:269:GLN:H	2.10	0.50
1:E:132:ARG:HB3	1:E:205:GLU:HB3	1.92	0.50
1:I:101:ASN:HD22	2:J:268:VAL:CG2	2.24	0.50
1:G:85:MET:O	1:G:110:ARG:HA	2.11	0.50
2:B:184:THR:HG22	2:B:249:SER:CA	2.40	0.50
2:N:66:GLY:HA3	2:N:119:ALA:O	2.11	0.50
2:N:215:PHE:C	2:N:215:PHE:CD2	2.84	0.50
1:C:133:PHE:CD2	1:C:140:LEU:HD21	2.31	0.50
2:F:184:THR:HG22	2:F:249:SER:CA	2.42	0.50
2:H:163:VAL:CG1	2:H:183:LEU:HD21	2.41	0.50
1:C:194:GLY:O	2:D:158:THR:HG21	2.12	0.50
1:A:194:GLY:O	2:B:158:THR:HG21	2.11	0.50
1:G:114:TYR:CE2	1:G:149:TYR:HB2	2.47	0.50
1:O:66:ARG:HG2	1:O:66:ARG:HH11	1.77	0.50
2:H:166:ARG:O	2:H:167:ASP:HB2	2.12	0.50
1:I:67:ILE:N	1:I:67:ILE:HD12	2.26	0.50
2:B:126:ILE:CD1	2:B:150:ALA:HB2	2.24	0.50
2:L:207:SER:O	2:L:224:GLN:HG3	2.10	0.50
2:F:211:ASN:ND2	2:F:269:GLN:H	2.10	0.50
1:A:94:ASP:CG	2:B:168:VAL:HG11	2.32	0.50
1:G:186:THR:CG2	1:G:199:LYS:NZ	2.75	0.50
1:E:12:PRO:HD2	1:E:15:GLN:HG3	1.92	0.50
1:M:149:TYR:CD2	1:M:168:PRO:HA	2.47	0.50
1:C:85:MET:O	1:C:110:ARG:HA	2.11	0.50
2:J:66:GLY:HA3	2:J:119:ALA:O	2.11	0.50
1:E:194:GLY:O	2:F:158:THR:HG21	2.12	0.50
2:H:22:VAL:HG23	2:H:22:VAL:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:67:VAL:CG2	2:H:126:ILE:HG12	2.42	0.50
1:O:47:ARG:HH22	1:O:74:GLN:HB2	1.76	0.50
2:F:174:ASP:O	2:F:176:PRO:HD2	2.12	0.50
2:P:126:ILE:HD12	2:P:148:ILE:HG22	1.94	0.50
2:J:190:SER:HA	2:J:244:GLY:HA2	1.93	0.50
1:K:9:VAL:O	1:K:113:LEU:HA	2.11	0.50
1:O:9:VAL:O	1:O:113:LEU:HA	2.11	0.50
2:D:185:VAL:HG23	2:D:243:VAL:HG11	1.93	0.50
2:D:50:GLU:H	2:D:50:GLU:CD	2.15	0.50
1:C:132:ARG:HB3	1:C:205:GLU:HB3	1.92	0.49
2:F:173:PRO:HG3	2:F:179:VAL:CG1	2.39	0.49
2:B:211:ASN:HD21	2:B:269:GLN:H	1.57	0.49
2:B:211:ASN:ND2	2:B:269:GLN:H	2.10	0.49
1:O:149:TYR:CD2	1:O:168:PRO:HA	2.47	0.49
1:C:11:TYR:CE2	1:C:69:ASP:HB2	2.47	0.49
1:G:22:VAL:CG2	1:G:65:LEU:HG	2.42	0.49
2:L:190:SER:HA	2:L:244:GLY:HA2	1.93	0.49
1:K:79:ARG:HB3	1:K:170:MET:HE3	1.93	0.49
1:E:142:LEU:HD22	1:E:142:LEU:H	1.77	0.49
2:B:22:VAL:HG23	2:B:22:VAL:O	2.11	0.49
1:M:67:ILE:N	1:M:67:ILE:HD12	2.26	0.49
2:B:50:GLU:CD	2:B:50:GLU:H	2.14	0.49
2:J:225:LEU:O	2:J:231:ILE:HG23	2.12	0.49
1:I:47:ARG:HH22	1:I:74:GLN:HB2	1.76	0.49
1:G:94:ASP:CG	2:H:168:VAL:HG11	2.33	0.49
1:E:94:ASP:CG	2:F:168:VAL:HG11	2.32	0.49
1:I:149:TYR:CD2	1:I:168:PRO:HA	2.47	0.49
1:A:12:PRO:HD2	1:A:15:GLN:HG3	1.93	0.49
2:L:271:ILE:HD12	2:L:271:ILE:N	2.28	0.49
2:F:227:ARG:HA	2:F:251:GLY:O	2.12	0.49
2:B:163:VAL:HG13	2:B:183:LEU:HD21	1.95	0.49
1:C:186:THR:CG2	1:C:199:LYS:NZ	2.75	0.49
2:J:253:THR:HG22	2:J:255:ASN:ND2	2.21	0.49
2:N:227:ARG:HA	2:N:251:GLY:O	2.13	0.49
2:P:145:VAL:HG12	2:P:146:TRP:N	2.27	0.49
2:J:145:VAL:HG12	2:J:146:TRP:N	2.27	0.49
2:N:208:ILE:HG23	2:N:257:ALA:CB	2.40	0.49
1:K:149:TYR:CD2	1:K:168:PRO:HA	2.47	0.49
2:P:271:ILE:N	2:P:271:ILE:HD12	2.28	0.49
1:K:11:TYR:CZ	1:K:69:ASP:HB2	2.47	0.49
2:J:75:VAL:HG13	2:J:75:VAL:O	2.11	0.49
2:N:225:LEU:O	2:N:231:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:41:ASP:HB2	1:K:43:VAL:HG12	1.94	0.49
1:O:41:ASP:HB2	1:O:43:VAL:HG12	1.94	0.49
1:A:156:ASN:C	1:A:158:GLY:H	2.16	0.49
2:L:21:TYR:CB	2:L:151:ASN:HD21	2.24	0.49
2:J:164:SER:HB2	2:J:184:THR:O	2.11	0.49
1:G:194:GLY:O	2:H:158:THR:HG21	2.11	0.49
2:H:163:VAL:HG13	2:H:183:LEU:HD21	1.94	0.49
1:M:9:VAL:O	1:M:113:LEU:HA	2.11	0.49
1:A:132:ARG:HB3	1:A:205:GLU:HB3	1.93	0.49
2:N:145:VAL:HG12	2:N:146:TRP:N	2.27	0.49
1:M:140:LEU:HD22	1:M:142:LEU:HD22	1.95	0.49
2:L:164:SER:HB2	2:L:184:THR:O	2.11	0.49
1:I:11:TYR:CZ	1:I:69:ASP:HB2	2.47	0.49
1:O:11:TYR:CZ	1:O:69:ASP:HB2	2.47	0.49
2:D:163:VAL:CG1	2:D:183:LEU:HD21	2.43	0.49
2:P:227:ARG:HA	2:P:251:GLY:O	2.13	0.49
2:P:66:GLY:HA3	2:P:119:ALA:O	2.12	0.49
1:M:98:LEU:HD13	1:M:98:LEU:C	2.33	0.49
1:G:132:ARG:HB3	1:G:205:GLU:HB3	1.93	0.49
1:M:101:ASN:HD22	2:N:268:VAL:CG2	2.23	0.49
1:E:13:ALA:HB3	1:E:118:ALA:H	1.76	0.49
1:O:39:ASN:CG	1:O:43:VAL:HG13	2.33	0.49
2:J:126:ILE:HD12	2:J:148:ILE:HG22	1.94	0.49
1:K:140:LEU:HD22	1:K:142:LEU:HD22	1.95	0.49
1:O:140:LEU:HD22	1:O:142:LEU:HD22	1.95	0.49
1:A:12:PRO:HB2	1:A:15:GLN:HG2	1.93	0.49
2:N:271:ILE:HD12	2:N:271:ILE:N	2.27	0.49
2:D:185:VAL:HG11	2:D:276:PHE:CE2	2.48	0.49
1:E:1:GLY:N	1:E:26:ASP:CG	2.66	0.49
2:J:45:HIS:HB3	2:J:100:ASP:HA	1.95	0.49
2:B:67:VAL:CG2	2:B:126:ILE:HG12	2.42	0.49
2:H:185:VAL:HG11	2:H:276:PHE:CE2	2.48	0.49
2:F:185:VAL:HG11	2:F:276:PHE:CE2	2.48	0.49
2:P:225:LEU:O	2:P:231:ILE:HG23	2.13	0.49
2:F:173:PRO:O	2:F:256:TYR:HE1	1.96	0.49
1:I:47:ARG:HH22	1:I:74:GLN:NE2	1.92	0.49
2:P:163:VAL:HA	2:P:185:VAL:CG2	2.35	0.49
1:G:156:ASN:C	1:G:158:GLY:H	2.16	0.49
2:L:270:SER:C	2:L:271:ILE:HD12	2.33	0.49
2:J:271:ILE:N	2:J:271:ILE:HD12	2.27	0.49
1:M:11:TYR:CZ	1:M:69:ASP:HB2	2.47	0.49
2:F:163:VAL:CG1	2:F:183:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:163:VAL:HG13	2:D:183:LEU:HD21	1.95	0.49
1:K:98:LEU:HD13	1:K:98:LEU:C	2.33	0.49
1:M:39:ASN:HB3	1:M:45:ASP:OD2	2.13	0.48
1:I:39:ASN:CG	1:I:43:VAL:HG13	2.32	0.48
2:H:211:ASN:ND2	2:H:211:ASN:C	2.66	0.48
1:I:27:GLU:HA	1:I:60:LYS:CG	2.43	0.48
1:I:140:LEU:HD22	1:I:142:LEU:HD22	1.95	0.48
2:J:34:LEU:HD12	2:J:35:VAL:N	2.21	0.48
1:C:12:PRO:HD2	1:C:15:GLN:HG3	1.94	0.48
2:N:267:ASN:HB3	2:N:269:GLN:HE21	1.78	0.48
2:J:270:SER:C	2:J:271:ILE:HD12	2.33	0.48
2:H:227:ARG:HA	2:H:251:GLY:O	2.13	0.48
2:L:131:LEU:HD23	2:L:131:LEU:C	2.33	0.48
2:F:66:GLY:HA3	2:F:119:ALA:O	2.13	0.48
1:K:39:ASN:HB3	1:K:45:ASP:OD2	2.13	0.48
2:J:202:ALA:HB2	2:J:210:THR:CG2	2.34	0.48
2:L:126:ILE:HD12	2:L:148:ILE:HG22	1.95	0.48
2:N:164:SER:O	2:N:183:LEU:HD23	2.13	0.48
1:K:101:ASN:HD22	2:L:268:VAL:CG2	2.24	0.48
2:P:267:ASN:HB3	2:P:269:GLN:HE21	1.78	0.48
1:G:13:ALA:HB3	1:G:118:ALA:H	1.76	0.48
2:P:75:VAL:O	2:P:75:VAL:HG13	2.13	0.48
2:H:66:GLY:HA3	2:H:119:ALA:O	2.14	0.48
2:B:63:ALA:HB1	2:B:67:VAL:HG12	1.94	0.48
1:I:41:ASP:HB2	1:I:43:VAL:HG12	1.94	0.48
2:F:211:ASN:ND2	2:F:211:ASN:C	2.66	0.48
2:D:166:ARG:O	2:D:167:ASP:HB2	2.14	0.48
1:O:101:ASN:HD22	2:P:268:VAL:CG2	2.23	0.48
2:N:270:SER:C	2:N:271:ILE:HD12	2.33	0.48
2:P:270:SER:C	2:P:271:ILE:HD12	2.33	0.48
2:L:267:ASN:HB3	2:L:269:GLN:HE21	1.79	0.48
1:M:6:ALA:HB3	1:M:20:LEU:CD1	2.44	0.48
1:A:142:LEU:H	1:A:142:LEU:HD22	1.78	0.48
1:G:93:MET:CE	1:G:98:LEU:HD23	2.43	0.48
1:I:39:ASN:HB3	1:I:45:ASP:OD2	2.13	0.48
2:B:166:ARG:O	2:B:167:ASP:HB2	2.13	0.48
2:L:145:VAL:HG12	2:L:146:TRP:N	2.28	0.48
1:E:11:TYR:CE2	1:E:69:ASP:HB2	2.49	0.48
2:J:96:ASN:N	2:J:96:ASN:HD22	2.10	0.48
2:H:131:LEU:HB3	2:H:144:PHE:HB2	1.96	0.48
2:H:181:ILE:HB	2:H:252:LEU:HB2	1.96	0.48
2:P:215:PHE:CD2	2:P:215:PHE:C	2.84	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:39:ASN:CG	1:M:43:VAL:HG13	2.33	0.48
2:H:172:LEU:N	2:H:173:PRO:CD	2.75	0.48
2:D:33:ASN:ND2	2:D:110:THR:OG1	2.46	0.48
2:P:38:LEU:C	2:P:40:THR:N	2.67	0.48
2:P:45:HIS:HB3	2:P:100:ASP:HA	1.96	0.48
2:D:66:GLY:HA3	2:D:119:ALA:O	2.13	0.48
2:P:253:THR:HG22	2:P:255:ASN:ND2	2.22	0.48
1:O:39:ASN:HB3	1:O:45:ASP:OD2	2.13	0.48
1:A:71:THR:HG23	1:A:71:THR:O	2.14	0.48
2:D:136:ASN:C	2:D:136:ASN:ND2	2.67	0.48
2:J:17:SER:HB2	2:L:262:GLN:OE1	2.13	0.48
2:B:33:ASN:ND2	2:B:110:THR:OG1	2.46	0.48
1:G:11:TYR:CE2	1:G:69:ASP:HB2	2.48	0.48
2:N:131:LEU:C	2:N:131:LEU:HD23	2.34	0.48
1:K:6:ALA:HB3	1:K:20:LEU:CD1	2.43	0.48
2:B:181:ILE:HB	2:B:252:LEU:HB2	1.95	0.48
1:O:98:LEU:HD13	1:O:98:LEU:C	2.33	0.48
2:B:66:GLY:HA3	2:B:119:ALA:O	2.13	0.48
1:C:140:LEU:H	1:C:177:LEU:HB2	1.79	0.48
2:N:227:ARG:CD	2:N:232:ILE:HD11	2.44	0.48
2:L:225:LEU:O	2:L:231:ILE:HG23	2.12	0.48
2:L:227:ARG:CD	2:L:232:ILE:HD11	2.44	0.48
2:B:172:LEU:N	2:B:173:PRO:CD	2.76	0.48
1:M:27:GLU:HA	1:M:60:LYS:CG	2.43	0.48
2:F:166:ARG:O	2:F:167:ASP:HB2	2.14	0.48
2:N:17:SER:HB2	2:P:262:GLN:OE1	2.13	0.48
2:L:38:LEU:C	2:L:40:THR:N	2.67	0.48
2:L:45:HIS:HB3	2:L:100:ASP:HA	1.96	0.48
1:M:37:VAL:HG11	1:M:48:PHE:HB2	1.96	0.48
2:L:227:ARG:HA	2:L:251:GLY:O	2.13	0.48
2:D:173:PRO:O	2:D:256:TYR:HE1	1.97	0.48
1:G:140:LEU:H	1:G:177:LEU:HB2	1.78	0.48
1:E:186:THR:HG21	1:E:199:LYS:HZ1	1.79	0.48
1:E:140:LEU:H	1:E:177:LEU:HB2	1.78	0.48
1:O:79:ARG:HB3	1:O:170:MET:HE3	1.94	0.48
2:D:77:TYR:CE2	2:D:90:THR:HG21	2.49	0.48
2:D:173:PRO:HG3	2:D:179:VAL:CG1	2.40	0.48
1:A:186:THR:CG2	1:A:199:LYS:NZ	2.76	0.48
2:N:218:ALA:HA	2:N:264:THR:HB	1.96	0.48
2:P:164:SER:O	2:P:183:LEU:HD23	2.13	0.48
2:J:267:ASN:HB3	2:J:269:GLN:HE21	1.78	0.48
2:N:96:ASN:N	2:N:96:ASN:HD22	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1:GLY:N	1:E:26:ASP:OD1	2.46	0.48
1:K:37:VAL:HG11	1:K:48:PHE:HB2	1.96	0.48
1:I:133:PHE:HD2	1:I:140:LEU:HD21	1.79	0.48
2:L:96:ASN:ND2	2:L:96:ASN:H	2.11	0.48
2:D:227:ARG:HA	2:D:251:GLY:O	2.13	0.48
2:N:45:HIS:HB3	2:N:100:ASP:HA	1.95	0.48
2:L:75:VAL:O	2:L:75:VAL:HG13	2.14	0.48
1:M:41:ASP:HB2	1:M:43:VAL:HG12	1.94	0.47
2:H:173:PRO:O	2:H:256:TYR:HE1	1.97	0.47
1:G:71:THR:HG23	1:G:71:THR:O	2.13	0.47
1:E:156:ASN:C	1:E:158:GLY:H	2.17	0.47
1:E:186:THR:CG2	1:E:199:LYS:NZ	2.76	0.47
1:M:135:ARG:HH22	1:M:181:ALA:CB	2.27	0.47
2:L:164:SER:O	2:L:183:LEU:HD23	2.13	0.47
1:G:1:GLY:N	1:G:26:ASP:CG	2.68	0.47
1:C:134:ARG:NE	1:C:141:THR:HG21	2.28	0.47
2:B:173:PRO:O	2:B:256:TYR:HE1	1.98	0.47
1:K:39:ASN:CG	1:K:43:VAL:HG13	2.33	0.47
1:C:71:THR:O	1:C:71:THR:HG23	2.14	0.47
1:K:135:ARG:HH22	1:K:181:ALA:CB	2.27	0.47
1:I:135:ARG:HH22	1:I:181:ALA:CB	2.27	0.47
2:J:164:SER:O	2:J:183:LEU:HD23	2.14	0.47
2:J:131:LEU:C	2:J:131:LEU:HD23	2.34	0.47
2:D:181:ILE:HB	2:D:252:LEU:HB2	1.96	0.47
1:I:98:LEU:C	1:I:98:LEU:HD13	2.33	0.47
2:N:126:ILE:HD12	2:N:148:ILE:HG22	1.94	0.47
1:O:135:ARG:HH22	1:O:181:ALA:CB	2.27	0.47
2:P:155:VAL:HG12	2:P:157:PRO:CD	2.43	0.47
2:P:48:TYR:H	3:P:1607:MAN:H62	1.80	0.47
2:H:77:TYR:CE2	2:H:90:THR:HG21	2.49	0.47
2:J:38:LEU:C	2:J:40:THR:N	2.66	0.47
2:F:163:VAL:HG13	2:F:183:LEU:HD21	1.96	0.47
1:A:1:GLY:N	1:A:26:ASP:OD1	2.47	0.47
1:C:1:GLY:N	1:C:26:ASP:OD1	2.47	0.47
1:M:47:ARG:NH2	1:M:74:GLN:NE2	2.59	0.47
1:A:186:THR:HG21	1:A:199:LYS:HZ1	1.79	0.47
2:P:267:ASN:CB	2:P:269:GLN:HE21	2.28	0.47
2:D:184:THR:HG22	2:D:249:SER:CA	2.43	0.47
2:P:227:ARG:CD	2:P:232:ILE:HD11	2.44	0.47
1:I:6:ALA:HB3	1:I:20:LEU:CD1	2.44	0.47
2:N:75:VAL:O	2:N:75:VAL:HG13	2.14	0.47
1:E:71:THR:HG23	1:E:71:THR:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:218:ALA:HA	2:P:264:THR:HB	1.96	0.47
2:N:163:VAL:HA	2:N:185:VAL:CG2	2.36	0.47
2:L:218:ALA:HA	2:L:264:THR:HB	1.96	0.47
1:O:27:GLU:HA	1:O:60:LYS:CG	2.43	0.47
1:O:133:PHE:HD2	1:O:140:LEU:HD21	1.79	0.47
1:E:12:PRO:HB2	1:E:15:GLN:HG2	1.96	0.47
1:O:6:ALA:HB3	1:O:20:LEU:CD1	2.44	0.47
2:P:131:LEU:HD23	2:P:131:LEU:C	2.33	0.47
2:F:181:ILE:HB	2:F:252:LEU:HB2	1.97	0.47
1:C:114:TYR:CE2	1:C:149:TYR:HB2	2.50	0.47
1:E:114:TYR:CE2	1:E:149:TYR:HB2	2.49	0.47
1:K:178:PRO:O	1:K:179:SER:HB3	2.15	0.47
1:I:185:ILE:O	1:I:202:GLY:N	2.35	0.47
2:B:77:TYR:CE2	2:B:90:THR:HG21	2.50	0.47
1:A:11:TYR:CE2	1:A:69:ASP:HB2	2.50	0.47
2:J:227:ARG:CD	2:J:232:ILE:HD11	2.44	0.47
2:L:66:GLY:HA2	2:L:70:ASN:HD22	1.79	0.47
2:P:53:THR:H	2:P:136:ASN:ND2	2.13	0.47
2:B:60:ARG:CZ	2:B:60:ARG:HB2	2.45	0.47
1:C:141:THR:HB	1:C:174:THR:CG2	2.41	0.47
2:P:226:THR:CG2	2:P:253:THR:HB	2.43	0.47
2:N:226:THR:CG2	2:N:253:THR:HB	2.42	0.47
1:K:47:ARG:HH22	1:K:74:GLN:NE2	1.92	0.47
1:G:140:LEU:C	1:G:140:LEU:HD23	2.35	0.47
1:I:47:ARG:NH2	1:I:74:GLN:NE2	2.58	0.47
2:J:218:ALA:HA	2:J:264:THR:HB	1.96	0.47
1:O:178:PRO:O	1:O:179:SER:HB3	2.15	0.47
1:K:27:GLU:HA	1:K:60:LYS:CG	2.44	0.47
2:F:136:ASN:ND2	2:F:136:ASN:C	2.68	0.47
1:K:102:THR:H	2:L:269:GLN:HG2	1.80	0.47
1:M:11:TYR:OH	1:M:69:ASP:HB2	2.14	0.47
2:J:227:ARG:HA	2:J:251:GLY:O	2.13	0.47
2:P:66:GLY:HA2	2:P:70:ASN:HD22	1.79	0.47
1:C:142:LEU:HD22	1:C:142:LEU:H	1.78	0.47
2:D:240:LEU:HD21	2:D:250:LEU:HD22	1.96	0.47
2:L:179:VAL:O	2:L:179:VAL:HG23	2.15	0.47
1:C:33:ILE:O	1:C:54:LEU:HA	2.15	0.47
1:E:30:THR:HG22	1:E:31:TYR:N	2.30	0.47
1:A:30:THR:HG22	1:A:31:TYR:N	2.30	0.47
1:A:95:LYS:N	1:A:95:LYS:HD3	2.30	0.47
1:E:95:LYS:HD3	1:E:95:LYS:N	2.30	0.47
2:D:201:THR:HG23	2:D:203:ASP:H	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:178:PRO:O	1:M:179:SER:HB3	2.15	0.47
1:K:133:PHE:HD2	1:K:140:LEU:HD21	1.79	0.47
2:J:267:ASN:CB	2:J:269:GLN:HE21	2.28	0.47
1:K:11:TYR:OH	1:K:69:ASP:HB2	2.14	0.47
1:I:11:TYR:OH	1:I:69:ASP:HB2	2.14	0.47
2:N:1:PHE:HD1	2:N:144:PHE:CZ	2.33	0.47
1:G:1:GLY:N	1:G:26:ASP:OD1	2.48	0.47
1:G:142:LEU:HD22	1:G:142:LEU:H	1.78	0.47
2:D:195:TYR:CE1	2:D:238:VAL:HB	2.50	0.47
2:F:41:GLN:NE2	4:F:1523:HOH:O	2.48	0.47
2:H:41:GLN:NE2	4:H:1627:HOH:O	2.47	0.47
2:N:179:VAL:HG23	2:N:179:VAL:O	2.15	0.47
2:L:13:ILE:HG23	3:L:1504:MAN:C2	2.45	0.47
2:L:224:GLN:HE21	2:L:231:ILE:HD13	1.80	0.47
2:D:211:ASN:C	2:D:211:ASN:ND2	2.67	0.47
1:A:140:LEU:C	1:A:140:LEU:HD23	2.35	0.47
1:M:160:ARG:HG3	1:M:178:PRO:HG3	1.97	0.47
1:M:95:LYS:HD3	1:M:95:LYS:N	2.30	0.47
1:C:156:ASN:C	1:C:158:GLY:H	2.17	0.47
2:H:201:THR:HG23	2:H:203:ASP:H	1.80	0.47
1:A:140:LEU:H	1:A:177:LEU:HB2	1.79	0.47
2:D:192:ASN:HA	2:D:241:GLY:O	2.15	0.47
2:J:103:TRP:CE2	2:J:105:VAL:HG21	2.50	0.47
2:B:185:VAL:HG11	2:B:276:PHE:CE2	2.50	0.47
1:O:37:VAL:HG11	1:O:48:PHE:HB2	1.96	0.47
2:B:195:TYR:CE1	2:B:238:VAL:HB	2.50	0.47
1:I:37:VAL:HG11	1:I:48:PHE:HB2	1.96	0.47
1:M:61:LYS:O	1:M:62:GLU:HB2	2.15	0.47
2:L:253:THR:HG22	2:L:255:ASN:ND2	2.22	0.46
2:D:201:THR:CG2	2:D:206:ASN:HA	2.29	0.46
1:M:133:PHE:HD2	1:M:140:LEU:HD21	1.79	0.46
2:H:29:ASN:HA	4:H:1629:HOH:O	2.13	0.46
1:G:12:PRO:HD2	1:G:15:GLN:HG3	1.95	0.46
2:L:1:PHE:HD1	2:L:144:PHE:CZ	2.33	0.46
2:J:96:ASN:H	2:J:96:ASN:ND2	2.12	0.46
2:L:250:LEU:HD13	2:L:252:LEU:HD11	1.97	0.46
2:N:96:ASN:ND2	2:N:96:ASN:H	2.13	0.46
2:F:22:VAL:HG23	2:F:22:VAL:O	2.13	0.46
1:G:141:THR:HG23	1:G:174:THR:CG2	2.45	0.46
1:G:160:ARG:HG2	1:G:178:PRO:HG3	1.97	0.46
2:B:211:ASN:C	2:B:211:ASN:ND2	2.68	0.46
1:I:178:PRO:O	1:I:179:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:136:ASN:C	2:H:136:ASN:ND2	2.68	0.46
2:N:38:LEU:C	2:N:40:THR:N	2.67	0.46
1:O:11:TYR:OH	1:O:69:ASP:HB2	2.14	0.46
2:N:66:GLY:HA2	2:N:70:ASN:HD22	1.80	0.46
2:J:1:PHE:HD1	2:J:144:PHE:CZ	2.33	0.46
2:H:215:PHE:O	2:H:216:SER:C	2.54	0.46
2:N:53:THR:H	2:N:136:ASN:ND2	2.13	0.46
2:H:60:ARG:CZ	2:H:60:ARG:HB2	2.45	0.46
1:I:95:LYS:N	1:I:95:LYS:HD3	2.30	0.46
2:F:63:ALA:HB1	2:F:67:VAL:HG12	1.96	0.46
1:A:72:ASN:O	1:A:74:GLN:HG3	2.16	0.46
1:O:160:ARG:HG3	1:O:178:PRO:HG3	1.98	0.46
2:J:21:TYR:CB	2:J:151:ASN:HD21	2.24	0.46
1:G:12:PRO:HB2	1:G:15:GLN:HG2	1.96	0.46
1:A:94:ASP:C	1:A:96:SER:H	2.18	0.46
1:I:142:LEU:HB2	1:I:173:SER:O	2.16	0.46
2:B:136:ASN:C	2:B:136:ASN:ND2	2.68	0.46
1:A:12:PRO:CB	1:A:15:GLN:HG3	2.45	0.46
1:E:86:ASN:ND2	1:E:110:ARG:HB2	2.30	0.46
2:F:77:TYR:CE2	2:F:90:THR:HG21	2.51	0.46
1:C:1:GLY:H1	1:C:26:ASP:CG	2.19	0.46
2:H:195:TYR:CE1	2:H:238:VAL:HB	2.49	0.46
2:L:195:TYR:O	2:L:237:THR:HA	2.15	0.46
2:P:195:TYR:O	2:P:237:THR:HA	2.15	0.46
1:G:33:ILE:O	1:G:54:LEU:HA	2.15	0.46
2:B:113:SER:OG	2:P:81:SER:N	2.47	0.46
2:P:197:LEU:CD1	2:P:225:LEU:HD12	2.42	0.46
1:K:47:ARG:NH2	1:K:74:GLN:NE2	2.58	0.46
1:O:47:ARG:HH22	1:O:74:GLN:NE2	1.92	0.46
1:C:12:PRO:HB2	1:C:15:GLN:HG2	1.95	0.46
2:P:1:PHE:HD1	2:P:144:PHE:CZ	2.33	0.46
1:E:33:ILE:O	1:E:54:LEU:HA	2.14	0.46
1:A:28:ASN:O	1:A:29:SER:HB3	2.16	0.46
1:A:33:ILE:O	1:A:54:LEU:HA	2.15	0.46
2:F:88:SER:HA	4:F:1572:HOH:O	2.16	0.46
1:C:30:THR:HG22	1:C:31:TYR:N	2.30	0.46
2:F:60:ARG:CZ	2:F:60:ARG:HB2	2.45	0.46
1:C:140:LEU:C	1:C:140:LEU:HD23	2.35	0.46
2:F:201:THR:HG23	2:F:203:ASP:H	1.80	0.46
2:J:24:LEU:O	2:J:26:PRO:N	2.49	0.46
1:O:177:LEU:HD12	1:O:178:PRO:CD	2.40	0.46
2:N:19:ASN:HD21	2:P:219:GLN:CD	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:102:THR:H	2:J:269:GLN:HG2	1.80	0.46
1:M:102:THR:H	2:N:269:GLN:HG2	1.80	0.46
2:L:83:PRO:O	2:L:86:THR:HA	2.15	0.46
2:P:250:LEU:HD13	2:P:252:LEU:HD11	1.97	0.46
1:C:93:MET:CE	1:C:98:LEU:HD23	2.45	0.46
1:E:93:MET:CE	1:E:98:LEU:HD23	2.45	0.46
1:C:95:LYS:HD3	1:C:95:LYS:N	2.30	0.46
2:P:224:GLN:HE21	2:P:231:ILE:HD13	1.81	0.46
1:C:102:THR:C	2:D:171:THR:HG22	2.36	0.46
2:D:172:LEU:N	2:D:173:PRO:CD	2.77	0.46
1:K:39:ASN:HD21	1:K:43:VAL:CG1	2.18	0.46
1:C:72:ASN:O	1:C:74:GLN:HG3	2.16	0.46
1:A:138:ASN:CA	1:A:177:LEU:HB3	2.46	0.46
1:E:181:ALA:HB1	1:E:182:GLY:H	1.53	0.46
1:K:136:SER:HB2	1:K:139:SER:H	1.81	0.46
2:N:203:ASP:OD1	2:N:208:ILE:HD12	2.16	0.46
2:P:203:ASP:OD1	2:P:208:ILE:HD12	2.16	0.46
2:J:208:ILE:HG23	2:J:257:ALA:CB	2.40	0.46
1:I:79:ARG:HB3	1:I:170:MET:HE3	1.96	0.46
2:J:66:GLY:HA2	2:J:70:ASN:HD22	1.80	0.46
2:J:250:LEU:HD13	2:J:252:LEU:HD11	1.96	0.46
2:B:215:PHE:O	2:B:216:SER:C	2.54	0.46
2:B:135:ASN:HD21	2:B:138:ASN:HD21	1.63	0.46
2:J:53:THR:H	2:J:136:ASN:ND2	2.13	0.46
2:J:179:VAL:O	2:J:179:VAL:HG23	2.15	0.46
1:G:95:LYS:HD3	1:G:95:LYS:N	2.31	0.46
1:C:160:ARG:HG2	1:C:178:PRO:HG3	1.98	0.46
1:M:136:SER:HB2	1:M:139:SER:H	1.81	0.46
2:J:203:ASP:OD1	2:J:208:ILE:HD12	2.16	0.46
2:L:184:THR:OG1	2:L:247:ALA:HB1	2.16	0.46
1:K:12:PRO:HB2	1:K:15:GLN:HG3	1.97	0.46
1:G:86:ASN:ND2	1:G:110:ARG:HB2	2.31	0.46
2:N:103:TRP:CE2	2:N:105:VAL:HG21	2.51	0.46
2:P:96:ASN:H	2:P:96:ASN:ND2	2.12	0.46
2:D:131:LEU:HB3	2:D:144:PHE:HB2	1.97	0.46
2:B:13:ILE:HG13	4:B:1545:HOH:O	2.15	0.46
1:K:95:LYS:N	1:K:95:LYS:HD3	2.30	0.46
2:D:67:VAL:CG2	2:D:126:ILE:HG12	2.46	0.46
2:N:24:LEU:O	2:N:26:PRO:N	2.49	0.46
2:P:24:LEU:O	2:P:26:PRO:N	2.49	0.46
1:E:140:LEU:HD23	1:E:140:LEU:C	2.36	0.46
2:L:203:ASP:OD1	2:L:208:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:78:ASP:O	1:M:170:MET:HE1	2.16	0.46
1:O:102:THR:H	2:P:269:GLN:HG2	1.80	0.46
2:L:60:ARG:HG2	4:L:1505:HOH:O	2.14	0.46
2:P:83:PRO:O	2:P:86:THR:HA	2.16	0.46
2:J:175:TYR:N	2:J:176:PRO:CD	2.79	0.46
1:A:46:GLY:O	1:A:70:ALA:HB3	2.16	0.46
1:A:93:MET:CE	1:A:98:LEU:HD23	2.44	0.46
2:N:195:TYR:O	2:N:237:THR:HA	2.16	0.46
2:F:215:PHE:O	2:F:216:SER:C	2.54	0.46
1:G:72:ASN:O	1:G:74:GLN:HG3	2.16	0.46
1:A:160:ARG:HG2	1:A:178:PRO:HG3	1.98	0.46
1:K:142:LEU:HB2	1:K:173:SER:O	2.16	0.46
1:E:94:ASP:C	1:E:96:SER:H	2.19	0.46
2:N:267:ASN:CB	2:N:269:GLN:HE21	2.28	0.46
2:P:103:TRP:CE2	2:P:105:VAL:HG21	2.51	0.46
1:C:1:GLY:N	1:C:26:ASP:CG	2.70	0.46
1:O:57:MET:HA	1:O:61:LYS:CE	2.46	0.46
1:G:129:GLU:HG3	1:G:129:GLU:H	1.52	0.46
1:O:95:LYS:N	1:O:95:LYS:HD3	2.30	0.46
2:P:179:VAL:O	2:P:179:VAL:HG23	2.15	0.46
1:E:72:ASN:O	1:E:74:GLN:HG3	2.16	0.45
1:E:160:ARG:HG2	1:E:178:PRO:HG3	1.98	0.45
2:P:208:ILE:HG23	2:P:257:ALA:CB	2.40	0.45
1:A:86:ASN:ND2	1:A:110:ARG:HB2	2.31	0.45
2:P:184:THR:OG1	2:P:247:ALA:HB1	2.16	0.45
2:L:267:ASN:CB	2:L:269:GLN:HE21	2.28	0.45
1:E:191:ASN:ND2	1:E:195:ALA:HB3	2.31	0.45
2:N:83:PRO:O	2:N:86:THR:HA	2.17	0.45
2:N:250:LEU:HD13	2:N:252:LEU:HD11	1.97	0.45
2:L:250:LEU:CD1	2:L:252:LEU:HD11	2.47	0.45
1:M:57:MET:HA	1:M:61:LYS:CE	2.46	0.45
1:C:28:ASN:O	1:C:29:SER:HB3	2.15	0.45
1:I:57:MET:HA	1:I:61:LYS:CE	2.46	0.45
1:C:94:ASP:C	1:C:96:SER:H	2.19	0.45
2:L:34:LEU:HD12	2:L:35:VAL:N	2.21	0.45
2:J:250:LEU:CD1	2:J:252:LEU:HD11	2.47	0.45
1:E:28:ASN:O	1:E:29:SER:HB3	2.17	0.45
1:K:57:MET:HA	1:K:61:LYS:CE	2.46	0.45
1:C:141:THR:HA	1:C:174:THR:HA	1.98	0.45
2:J:224:GLN:HE21	2:J:231:ILE:HD13	1.80	0.45
1:A:186:THR:HB	1:A:199:LYS:NZ	2.32	0.45
1:I:136:SER:HB2	1:I:139:SER:H	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:175:TYR:N	2:P:176:PRO:CD	2.80	0.45
2:J:83:PRO:O	2:J:86:THR:HA	2.16	0.45
2:D:184:THR:HB	2:D:247:ALA:HB1	1.98	0.45
2:F:131:LEU:HB3	2:F:144:PHE:HB2	1.98	0.45
2:N:96:ASN:O	2:N:97:SER:HB2	2.17	0.45
1:G:28:ASN:O	1:G:28:ASN:ND2	2.49	0.45
2:D:215:PHE:O	2:D:216:SER:C	2.54	0.45
2:H:240:LEU:HD21	2:H:250:LEU:HD22	1.98	0.45
2:L:53:THR:H	2:L:136:ASN:ND2	2.13	0.45
1:C:162:LEU:HD21	1:C:178:PRO:CD	2.47	0.45
2:F:201:THR:CG2	2:F:206:ASN:HA	2.31	0.45
1:I:177:LEU:HD12	1:I:178:PRO:CD	2.40	0.45
1:M:142:LEU:HB2	1:M:173:SER:O	2.16	0.45
2:F:167:ASP:CG	2:F:168:VAL:HG12	2.37	0.45
1:G:186:THR:HB	1:G:199:LYS:NZ	2.31	0.45
2:P:154:VAL:HG12	2:P:155:VAL:N	2.32	0.45
1:I:12:PRO:HB2	1:I:15:GLN:HG3	1.97	0.45
2:J:155:VAL:HG12	2:J:157:PRO:CD	2.43	0.45
1:C:86:ASN:ND2	1:C:110:ARG:HB2	2.32	0.45
2:F:195:TYR:CE1	2:F:238:VAL:HB	2.51	0.45
1:A:156:ASN:O	1:A:185:ILE:HA	2.16	0.45
1:A:154:GLU:OE2	1:A:188:ARG:HD3	2.16	0.45
1:E:186:THR:CG2	1:E:199:LYS:HZ2	2.30	0.45
1:O:142:LEU:HB2	1:O:173:SER:O	2.16	0.45
2:N:184:THR:OG1	2:N:247:ALA:HB1	2.16	0.45
1:M:12:PRO:HB2	1:M:15:GLN:HG3	1.97	0.45
2:L:103:TRP:CE2	2:L:105:VAL:HG21	2.51	0.45
2:D:5:THR:CG2	2:D:8:GLY:H	2.29	0.45
2:D:158:THR:HG23	4:D:1617:HOH:O	2.15	0.45
2:P:250:LEU:CD1	2:P:252:LEU:HD11	2.47	0.45
2:N:195:TYR:HB2	2:N:275:THR:O	2.17	0.45
1:A:114:TYR:CE2	1:A:149:TYR:HB2	2.51	0.45
1:G:46:GLY:O	1:G:70:ALA:HB3	2.16	0.45
2:D:60:ARG:CZ	2:D:60:ARG:HB2	2.47	0.45
2:J:226:THR:CG2	2:J:253:THR:HB	2.42	0.45
1:G:102:THR:C	2:H:171:THR:HG22	2.37	0.45
1:I:160:ARG:HG3	1:I:178:PRO:HG3	1.98	0.45
1:O:61:LYS:O	1:O:62:GLU:HB2	2.15	0.45
1:C:138:ASN:CA	1:C:177:LEU:HB3	2.47	0.45
1:G:94:ASP:C	1:G:96:SER:H	2.18	0.45
1:K:160:ARG:HG3	1:K:178:PRO:HG3	1.98	0.45
1:E:138:ASN:CA	1:E:177:LEU:HB3	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:167:ASP:OD1	2:F:168:VAL:HG12	2.17	0.45
1:C:167:VAL:HA	1:C:168:PRO:HD2	1.77	0.45
1:G:122:LEU:HD12	1:G:122:LEU:C	2.37	0.45
2:B:184:THR:HB	2:B:247:ALA:HB1	1.98	0.45
1:I:61:LYS:O	1:I:62:GLU:HB2	2.16	0.45
1:O:144:ASN:HB3	1:O:167:VAL:HG12	1.99	0.45
1:E:102:THR:C	2:F:171:THR:HG22	2.36	0.45
1:G:125:ASP:OD1	1:G:126:GLN:N	2.50	0.45
1:O:144:ASN:HB3	1:O:167:VAL:CG1	2.47	0.45
1:C:46:GLY:O	1:C:70:ALA:HB3	2.16	0.45
1:I:144:ASN:HB3	1:I:167:VAL:HG12	1.99	0.45
2:J:195:TYR:O	2:J:237:THR:HA	2.16	0.45
2:J:195:TYR:HB2	2:J:275:THR:O	2.16	0.45
2:D:4:LYS:NZ	2:D:4:LYS:HB2	2.31	0.45
2:N:227:ARG:NE	2:N:232:ILE:HD11	2.32	0.45
1:M:47:ARG:HH22	1:M:74:GLN:NE2	1.92	0.45
1:E:186:THR:HB	1:E:199:LYS:NZ	2.32	0.45
2:H:167:ASP:CG	2:H:168:VAL:HG12	2.38	0.45
1:M:149:TYR:CD1	1:M:169:PRO:HD3	2.52	0.45
2:J:96:ASN:O	2:J:97:SER:HB2	2.17	0.45
1:K:61:LYS:O	1:K:62:GLU:HB2	2.16	0.45
1:C:201:THR:O	1:C:203:VAL:HG23	2.17	0.45
2:B:240:LEU:HD21	2:B:250:LEU:HD22	1.97	0.45
2:F:118:VAL:O	2:F:118:VAL:HG12	2.17	0.45
2:D:38:LEU:C	2:D:40:THR:N	2.69	0.45
2:H:201:THR:CB	2:H:206:ASN:ND2	2.81	0.45
1:O:47:ARG:NH2	1:O:74:GLN:NE2	2.58	0.45
1:G:141:THR:HA	1:G:174:THR:HA	1.99	0.45
2:L:24:LEU:O	2:L:26:PRO:N	2.49	0.45
1:O:136:SER:HB2	1:O:139:SER:H	1.81	0.45
1:C:144:ASN:HB3	1:C:167:VAL:HG12	1.98	0.45
2:L:96:ASN:O	2:L:97:SER:HB2	2.17	0.45
1:A:1:GLY:N	1:A:26:ASP:CG	2.69	0.45
2:N:197:LEU:CD1	2:N:225:LEU:HD12	2.43	0.44
1:A:186:THR:CG2	1:A:199:LYS:HZ2	2.30	0.44
1:E:156:ASN:O	1:E:185:ILE:HA	2.17	0.44
2:N:42:ILE:HG23	2:N:146:TRP:CH2	2.52	0.44
1:C:82:LEU:HD12	1:C:83:PHE:H	1.82	0.44
2:P:227:ARG:NE	2:P:232:ILE:HD11	2.32	0.44
2:P:195:TYR:HB2	2:P:275:THR:O	2.16	0.44
2:F:38:LEU:C	2:F:40:THR:N	2.70	0.44
1:G:30:THR:HG22	1:G:31:TYR:N	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:46:GLY:O	1:E:70:ALA:HB3	2.17	0.44
1:C:156:ASN:O	1:C:185:ILE:HA	2.16	0.44
1:C:154:GLU:OE2	1:C:188:ARG:HD3	2.17	0.44
2:N:253:THR:HG22	2:N:255:ASN:ND2	2.22	0.44
1:A:102:THR:C	2:B:171:THR:HG22	2.37	0.44
1:E:71:THR:O	1:E:73:ASN:N	2.51	0.44
2:F:136:ASN:N	2:F:136:ASN:HD22	2.15	0.44
2:J:184:THR:OG1	2:J:247:ALA:HB1	2.17	0.44
2:J:154:VAL:HG12	2:J:155:VAL:N	2.32	0.44
1:O:82:LEU:HB2	1:O:149:TYR:CE1	2.53	0.44
1:A:144:ASN:HB3	1:A:167:VAL:HG12	1.98	0.44
1:G:144:ASN:HB3	1:G:167:VAL:HG12	1.98	0.44
2:P:96:ASN:O	2:P:97:SER:HB2	2.17	0.44
1:G:28:ASN:O	1:G:29:SER:HB3	2.16	0.44
1:E:201:THR:O	1:E:203:VAL:HG23	2.18	0.44
2:N:224:GLN:HE21	2:N:231:ILE:HD13	1.80	0.44
1:I:39:ASN:OD1	1:I:43:VAL:HG13	2.18	0.44
1:K:177:LEU:HD12	1:K:178:PRO:CD	2.40	0.44
2:J:42:ILE:HG23	2:J:146:TRP:CH2	2.53	0.44
2:N:154:VAL:HG12	2:N:155:VAL:N	2.32	0.44
2:N:175:TYR:N	2:N:176:PRO:CD	2.80	0.44
1:I:57:MET:HA	1:I:61:LYS:HE3	2.00	0.44
1:I:144:ASN:HB3	1:I:167:VAL:CG1	2.48	0.44
1:O:85:MET:O	1:O:110:ARG:HA	2.17	0.44
1:K:85:MET:O	1:K:110:ARG:HA	2.17	0.44
1:K:71:THR:HG23	1:K:71:THR:O	2.17	0.44
2:B:201:THR:HG23	2:B:203:ASP:H	1.82	0.44
2:F:172:LEU:N	2:F:173:PRO:CD	2.76	0.44
2:N:59:GLN:HG3	2:N:132:ARG:HD3	2.00	0.44
2:L:155:VAL:HG12	2:L:157:PRO:CD	2.43	0.44
1:O:186:THR:HB	1:O:199:LYS:NZ	2.32	0.44
2:N:250:LEU:CD1	2:N:252:LEU:HD11	2.47	0.44
1:I:190:ILE:HD12	2:J:279:GLN:HG2	1.99	0.44
2:H:135:ASN:HD21	2:H:138:ASN:HD21	1.64	0.44
1:I:85:MET:O	1:I:110:ARG:HA	2.17	0.44
1:G:201:THR:O	1:G:203:VAL:HG23	2.18	0.44
1:A:47:ARG:NH2	1:A:74:GLN:HB2	2.33	0.44
1:E:141:THR:HA	1:E:174:THR:HA	2.00	0.44
1:O:12:PRO:HD2	1:O:15:GLN:HG3	1.99	0.44
1:I:82:LEU:HB2	1:I:149:TYR:CE1	2.52	0.44
2:L:267:ASN:OD1	2:L:269:GLN:NE2	2.51	0.44
2:P:61:GLY:HA3	2:P:86:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:190:ILE:HD12	2:N:279:GLN:HG2	2.00	0.44
1:C:28:ASN:O	1:C:28:ASN:ND2	2.51	0.44
1:M:144:ASN:HB3	1:M:167:VAL:CG1	2.47	0.44
1:G:138:ASN:CA	1:G:177:LEU:HB3	2.48	0.44
1:A:177:LEU:HA	1:A:178:PRO:HD2	1.88	0.44
2:P:58:LEU:H	2:P:90:THR:HG21	1.79	0.44
1:G:154:GLU:OE2	1:G:188:ARG:HD3	2.17	0.44
1:M:82:LEU:HB2	1:M:149:TYR:CE1	2.53	0.44
1:E:122:LEU:HD12	1:E:122:LEU:C	2.38	0.44
2:N:168:VAL:O	2:N:168:VAL:HG13	2.18	0.44
1:I:186:THR:HB	1:I:199:LYS:NZ	2.32	0.44
2:L:195:TYR:HB2	2:L:275:THR:O	2.17	0.44
1:O:71:THR:O	1:O:71:THR:HG23	2.18	0.44
1:M:45:ASP:OD1	1:M:47:ARG:HB2	2.18	0.44
1:K:39:ASN:OD1	1:K:43:VAL:HG13	2.18	0.44
2:P:202:ALA:HB2	2:P:210:THR:CG2	2.34	0.44
1:C:71:THR:O	1:C:73:ASN:N	2.51	0.44
1:E:47:ARG:NH2	1:E:74:GLN:HB2	2.32	0.44
1:K:179:SER:C	1:K:181:ALA:H	2.20	0.44
2:P:42:ILE:HG23	2:P:146:TRP:CH2	2.53	0.44
2:H:192:ASN:HA	2:H:241:GLY:O	2.18	0.44
1:O:12:PRO:HB2	1:O:15:GLN:HG3	1.98	0.44
1:O:149:TYR:CD1	1:O:169:PRO:HD3	2.52	0.44
1:K:78:ASP:O	1:K:170:MET:HE1	2.18	0.44
2:N:267:ASN:OD1	2:N:269:GLN:NE2	2.51	0.44
2:J:168:VAL:HG13	2:J:168:VAL:O	2.18	0.44
1:E:123:PRO:HA	1:E:124:PRO:HD2	1.84	0.44
2:P:267:ASN:OD1	2:P:269:GLN:NE2	2.50	0.44
2:J:61:GLY:HA3	2:J:86:THR:HG23	1.99	0.44
2:B:184:THR:HA	2:B:248:VAL:O	2.18	0.44
1:M:186:THR:HB	1:M:199:LYS:NZ	2.33	0.44
2:D:5:THR:HG22	2:D:9:THR:N	2.32	0.44
2:J:44:CYS:O	2:J:101:LYS:N	2.50	0.44
2:P:211:ASN:HD22	2:P:212:THR:N	2.16	0.44
2:J:211:ASN:HD22	2:J:212:THR:N	2.16	0.44
1:I:71:THR:HG23	1:I:71:THR:O	2.18	0.44
2:H:4:LYS:HB2	2:H:4:LYS:NZ	2.33	0.44
1:C:186:THR:HB	1:C:199:LYS:NZ	2.32	0.44
1:G:162:LEU:HD21	1:G:178:PRO:CD	2.48	0.44
2:P:59:GLN:HG3	2:P:132:ARG:HD3	2.00	0.44
2:B:167:ASP:OD1	2:B:168:VAL:HG12	2.18	0.44
2:D:167:ASP:OD1	2:D:168:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:190:ILE:HD12	2:L:279:GLN:HG2	2.00	0.44
2:P:21:TYR:CB	2:P:151:ASN:HD21	2.24	0.44
1:C:12:PRO:CB	1:C:15:GLN:HG3	2.45	0.44
1:A:122:LEU:C	1:A:122:LEU:HD12	2.38	0.44
1:A:191:ASN:ND2	1:A:195:ALA:HB3	2.33	0.44
1:O:190:ILE:HD12	2:P:279:GLN:HG2	2.00	0.44
1:M:144:ASN:HB3	1:M:167:VAL:HG12	1.99	0.44
2:L:211:ASN:HD22	2:L:212:THR:N	2.16	0.44
2:L:227:ARG:NE	2:L:232:ILE:HD11	2.32	0.44
1:K:45:ASP:OD1	1:K:47:ARG:HB2	2.18	0.44
2:L:59:GLN:HG3	2:L:132:ARG:HD3	2.00	0.44
1:A:187:TYR:CD1	1:A:187:TYR:C	2.91	0.44
1:E:154:GLU:OE2	1:E:188:ARG:HD3	2.18	0.44
1:I:160:ARG:HG2	1:I:178:PRO:HG3	2.00	0.44
2:L:42:ILE:HG23	2:L:146:TRP:CH2	2.53	0.44
1:G:156:ASN:O	1:G:185:ILE:HA	2.17	0.44
1:K:149:TYR:CD1	1:K:169:PRO:HD3	2.52	0.44
2:J:95:TYR:HH	2:J:103:TRP:HA	1.83	0.44
2:F:184:THR:HB	2:F:247:ALA:HB1	1.98	0.44
2:H:38:LEU:C	2:H:40:THR:N	2.71	0.44
1:K:144:ASN:HB3	1:K:167:VAL:HG12	1.99	0.44
1:M:71:THR:O	1:M:71:THR:HG23	2.18	0.44
1:C:47:ARG:NH2	1:C:74:GLN:HB2	2.33	0.43
1:A:162:LEU:HD21	1:A:178:PRO:CD	2.47	0.43
1:E:162:LEU:HD21	1:E:178:PRO:CD	2.48	0.43
2:J:19:ASN:HD21	2:L:219:GLN:CD	2.21	0.43
2:L:154:VAL:HG12	2:L:155:VAL:N	2.32	0.43
2:L:175:TYR:N	2:L:176:PRO:CD	2.80	0.43
2:N:61:GLY:HA3	2:N:86:THR:HG23	2.00	0.43
1:K:186:THR:HB	1:K:199:LYS:NZ	2.32	0.43
1:K:24:ASN:HB2	1:K:57:MET:HE3	2.00	0.43
2:L:8:GLY:O	2:L:9:THR:C	2.57	0.43
1:E:155:LEU:HD12	1:E:187:TYR:HB3	2.01	0.43
1:O:160:ARG:HG2	1:O:178:PRO:HG3	2.00	0.43
2:J:41:GLN:O	2:J:42:ILE:HG13	2.18	0.43
1:K:82:LEU:HB2	1:K:149:TYR:CE1	2.53	0.43
2:D:184:THR:HA	2:D:248:VAL:O	2.18	0.43
2:H:184:THR:HB	2:H:247:ALA:HB1	1.99	0.43
1:E:31:TYR:O	1:E:56:ALA:HA	2.18	0.43
2:L:135:ASN:ND2	3:L:1504:MAN:O4	2.52	0.43
2:H:118:VAL:HG12	2:H:118:VAL:O	2.18	0.43
2:N:211:ASN:HD22	2:N:212:THR:N	2.16	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:201:THR:CB	2:F:206:ASN:ND2	2.81	0.43
2:L:67:VAL:HG21	2:L:126:ILE:CG2	2.35	0.43
2:N:58:LEU:H	2:N:90:THR:HG21	1.80	0.43
2:J:267:ASN:OD1	2:J:269:GLN:NE2	2.51	0.43
2:H:184:THR:HA	2:H:248:VAL:O	2.18	0.43
2:J:1:PHE:CD1	2:J:133:GLN:HG3	2.53	0.43
2:P:1:PHE:CD1	2:P:133:GLN:HG3	2.53	0.43
2:P:192:ASN:HA	2:P:241:GLY:O	2.18	0.43
2:H:5:THR:CG2	2:H:8:GLY:H	2.31	0.43
1:K:185:ILE:O	1:K:202:GLY:N	2.35	0.43
2:L:41:GLN:O	2:L:42:ILE:HG13	2.18	0.43
2:D:262:GLN:CA	2:D:262:GLN:HE21	2.25	0.43
1:A:125:ASP:OD1	1:A:126:GLN:N	2.51	0.43
2:L:30:VAL:HG23	2:L:156:VAL:CG1	2.49	0.43
2:N:30:VAL:HG23	2:N:156:VAL:CG1	2.49	0.43
1:O:57:MET:HA	1:O:61:LYS:HE3	2.00	0.43
1:M:50:VAL:HG12	1:M:51:THR:N	2.34	0.43
1:O:39:ASN:OD1	1:O:43:VAL:HG13	2.18	0.43
2:D:167:ASP:CG	2:D:168:VAL:HG12	2.37	0.43
1:K:52:PRO:HG2	1:K:55:PHE:CE2	2.53	0.43
1:O:78:ASP:O	1:O:170:MET:HE1	2.18	0.43
1:E:144:ASN:HB3	1:E:167:VAL:HG12	1.98	0.43
2:J:30:VAL:HG23	2:J:156:VAL:CG1	2.48	0.43
1:K:144:ASN:HB3	1:K:167:VAL:CG1	2.47	0.43
1:M:85:MET:O	1:M:110:ARG:HA	2.18	0.43
1:M:39:ASN:OD1	1:M:43:VAL:HG13	2.18	0.43
2:H:5:THR:HG22	2:H:9:THR:N	2.33	0.43
1:G:132:ARG:C	1:G:133:PHE:CD1	2.92	0.43
2:H:167:ASP:OD1	2:H:168:VAL:HG12	2.18	0.43
2:N:41:GLN:O	2:N:42:ILE:HG13	2.19	0.43
1:I:135:ARG:NH2	1:I:181:ALA:CB	2.82	0.43
2:P:41:GLN:O	2:P:42:ILE:HG13	2.18	0.43
2:N:21:TYR:CB	2:N:151:ASN:HD21	2.24	0.43
1:M:182:GLY:O	1:M:183:SER:CB	2.65	0.43
1:I:149:TYR:CG	1:I:169:PRO:HD3	2.54	0.43
1:I:149:TYR:CD1	1:I:169:PRO:HD3	2.52	0.43
2:B:221:VAL:HG12	2:B:222:GLY:N	2.33	0.43
1:G:168:PRO:HA	1:G:169:PRO:HD3	1.87	0.43
2:J:227:ARG:NE	2:J:232:ILE:HD11	2.33	0.43
1:A:28:ASN:ND2	1:A:28:ASN:O	2.51	0.43
1:G:155:LEU:HD12	1:G:187:TYR:HB3	2.01	0.43
1:A:201:THR:O	1:A:203:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:186:THR:CG2	1:C:199:LYS:HZ2	2.32	0.43
1:A:141:THR:HA	1:A:174:THR:HA	1.99	0.43
1:O:135:ARG:NH2	1:O:181:ALA:CB	2.81	0.43
1:K:135:ARG:NH2	1:K:181:ALA:CB	2.82	0.43
1:K:135:ARG:NH2	1:K:181:ALA:HB1	2.34	0.43
2:L:208:ILE:HG23	2:L:257:ALA:CB	2.40	0.43
2:L:192:ASN:HA	2:L:241:GLY:O	2.19	0.43
2:N:155:VAL:HG12	2:N:157:PRO:CD	2.43	0.43
2:N:30:VAL:HG12	2:N:31:GLY:N	2.33	0.43
1:E:125:ASP:OD1	1:E:126:GLN:N	2.51	0.43
2:P:168:VAL:HG13	2:P:168:VAL:O	2.18	0.43
1:O:13:ALA:HB3	1:O:118:ALA:H	1.84	0.43
2:F:184:THR:HA	2:F:248:VAL:O	2.18	0.43
1:O:188:ARG:NH1	1:O:199:LYS:N	2.67	0.43
2:J:192:ASN:HA	2:J:241:GLY:O	2.19	0.43
2:J:241:GLY:O	2:J:243:VAL:HG23	2.19	0.43
2:J:122:ALA:N	2:J:153:ASP:OD1	2.52	0.43
2:B:38:LEU:C	2:B:40:THR:N	2.72	0.43
1:K:41:ASP:C	1:K:43:VAL:H	2.22	0.43
1:G:47:ARG:NH2	1:G:74:GLN:HB2	2.31	0.43
1:A:47:ARG:NH2	1:A:74:GLN:NE2	2.54	0.43
1:A:132:ARG:C	1:A:133:PHE:CD1	2.92	0.43
1:E:187:TYR:C	1:E:187:TYR:CD1	2.92	0.43
2:L:241:GLY:O	2:L:243:VAL:HG23	2.19	0.43
1:I:52:PRO:HG2	1:I:55:PHE:CE2	2.53	0.43
2:N:95:TYR:OH	2:N:103:TRP:CA	2.66	0.43
2:N:241:GLY:O	2:N:243:VAL:HG23	2.19	0.43
1:G:93:MET:HE1	1:G:98:LEU:HD23	2.00	0.43
1:A:31:TYR:O	1:A:56:ALA:HA	2.19	0.43
1:G:31:TYR:O	1:G:56:ALA:HA	2.19	0.43
2:J:197:LEU:CD1	2:J:225:LEU:HD12	2.42	0.43
1:O:45:ASP:OD1	1:O:47:ARG:HB2	2.19	0.43
2:B:167:ASP:CG	2:B:168:VAL:HG12	2.38	0.43
1:M:135:ARG:NH2	1:M:181:ALA:CB	2.81	0.43
1:K:177:LEU:HA	1:K:178:PRO:HD2	1.79	0.43
1:O:52:PRO:HG2	1:O:55:PHE:CE2	2.54	0.43
1:E:122:LEU:HD12	1:E:123:PRO:N	2.34	0.43
2:B:5:THR:CG2	2:B:8:GLY:H	2.32	0.43
1:M:57:MET:HA	1:M:61:LYS:HE3	2.00	0.43
1:C:31:TYR:O	1:C:56:ALA:HA	2.18	0.43
1:C:187:TYR:CD1	1:C:187:TYR:C	2.92	0.43
2:B:1:PHE:CG	2:B:133:GLN:HG3	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:212:THR:O	2:B:269:GLN:HB2	2.19	0.43
1:M:179:SER:C	1:M:181:ALA:H	2.20	0.43
1:M:135:ARG:NH2	1:M:181:ALA:HB1	2.34	0.43
1:K:160:ARG:HG2	1:K:178:PRO:HG3	2.00	0.43
1:C:125:ASP:OD1	1:C:126:GLN:N	2.52	0.43
1:G:122:LEU:HD12	1:G:123:PRO:N	2.34	0.43
2:H:116:GLY:HA2	2:H:189:LYS:CE	2.48	0.43
1:E:28:ASN:ND2	1:E:28:ASN:O	2.52	0.43
2:L:53:THR:H	2:L:136:ASN:HD21	1.67	0.43
2:D:38:LEU:C	2:D:40:THR:H	2.21	0.43
2:J:13:ILE:HG23	3:J:1605:MAN:C2	2.48	0.43
2:B:4:LYS:NZ	2:B:4:LYS:HB2	2.34	0.43
2:P:207:SER:HB3	2:P:233:PRO:HB3	2.01	0.42
2:L:126:ILE:HD11	2:L:150:ALA:HB2	2.01	0.42
2:P:126:ILE:HD11	2:P:150:ALA:HB2	2.01	0.42
1:M:160:ARG:HG2	1:M:178:PRO:HG3	2.01	0.42
1:O:135:ARG:NH2	1:O:181:ALA:HB1	2.34	0.42
1:I:12:PRO:HD2	1:I:15:GLN:HG3	2.00	0.42
1:G:38:GLU:OE1	1:G:110:ARG:NH2	2.46	0.42
2:H:221:VAL:HG12	2:H:222:GLY:N	2.34	0.42
2:B:111:PRO:HB3	2:B:156:VAL:HG21	2.01	0.42
1:M:24:ASN:HB2	1:M:57:MET:HE3	2.00	0.42
1:G:187:TYR:C	1:G:187:TYR:CD1	2.92	0.42
2:J:135:ASN:ND2	3:J:1605:MAN:O4	2.52	0.42
1:G:67:ILE:HD12	1:G:67:ILE:N	2.34	0.42
1:M:77:GLN:NE2	1:M:77:GLN:HA	2.34	0.42
2:H:126:ILE:CD1	2:H:150:ALA:HB2	2.26	0.42
1:M:39:ASN:HD21	1:M:43:VAL:CG1	2.18	0.42
1:O:41:ASP:C	1:O:43:VAL:H	2.22	0.42
2:J:59:GLN:HG3	2:J:132:ARG:HD3	2.00	0.42
1:I:136:SER:C	1:I:177:LEU:HD23	2.39	0.42
1:M:52:PRO:HG2	1:M:55:PHE:CE2	2.54	0.42
2:N:29:ASN:OD1	2:N:157:PRO:HD2	2.19	0.42
2:L:29:ASN:OD1	2:L:157:PRO:HD2	2.19	0.42
1:K:149:TYR:CG	1:K:169:PRO:HD3	2.54	0.42
2:P:122:ALA:N	2:P:153:ASP:OD1	2.52	0.42
1:O:31:TYR:O	1:O:56:ALA:HA	2.19	0.42
2:H:201:THR:HB	2:H:206:ASN:ND2	2.34	0.42
2:D:226:THR:HG22	2:D:255:ASN:HD21	1.84	0.42
1:A:155:LEU:HD12	1:A:187:TYR:HB3	2.01	0.42
1:K:136:SER:C	1:K:177:LEU:HD23	2.39	0.42
2:J:41:GLN:C	2:J:42:ILE:HG13	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:168:VAL:O	2:L:168:VAL:HG13	2.18	0.42
1:I:13:ALA:HB3	1:I:118:ALA:H	1.84	0.42
1:O:24:ASN:HB2	1:O:57:MET:HE3	2.00	0.42
1:C:117:PRO:O	1:C:120:LEU:HG	2.19	0.42
1:G:117:PRO:O	1:G:120:LEU:HG	2.19	0.42
1:O:50:VAL:HG12	1:O:51:THR:N	2.34	0.42
2:F:4:LYS:NZ	2:F:4:LYS:HB2	2.34	0.42
2:P:223:VAL:CG1	2:P:224:GLN:N	2.82	0.42
2:J:223:VAL:CG1	2:J:224:GLN:N	2.82	0.42
2:D:226:THR:CG2	2:D:255:ASN:HD21	2.32	0.42
1:O:134:ARG:HD2	1:O:141:THR:OG1	2.20	0.42
2:P:41:GLN:C	2:P:42:ILE:HG13	2.40	0.42
2:H:33:ASN:HA	2:H:33:ASN:HD22	1.59	0.42
2:P:29:ASN:OD1	2:P:157:PRO:HD2	2.20	0.42
1:G:10:ILE:O	1:G:12:PRO:HD3	2.19	0.42
2:P:30:VAL:HG23	2:P:156:VAL:CG1	2.49	0.42
1:G:191:ASN:ND2	1:G:195:ALA:HB3	2.32	0.42
2:L:61:GLY:HA3	2:L:86:THR:HG23	2.00	0.42
1:K:13:ALA:HB3	1:K:118:ALA:H	1.84	0.42
1:O:188:ARG:NH1	1:O:199:LYS:H	2.17	0.42
2:P:136:ASN:N	2:P:136:ASN:HD22	2.17	0.42
2:J:8:GLY:O	2:J:9:THR:C	2.57	0.42
1:K:50:VAL:HG12	1:K:51:THR:N	2.34	0.42
2:J:181:ILE:HA	2:J:182:PRO:HD3	1.93	0.42
2:F:240:LEU:HD21	2:F:250:LEU:HD22	2.00	0.42
1:M:41:ASP:C	1:M:43:VAL:H	2.22	0.42
1:I:45:ASP:OD1	1:I:47:ARG:HB2	2.18	0.42
1:O:179:SER:C	1:O:181:ALA:H	2.21	0.42
2:H:136:ASN:N	2:H:136:ASN:HD22	2.18	0.42
2:F:192:ASN:HA	2:F:241:GLY:O	2.19	0.42
1:M:12:PRO:HD2	1:M:15:GLN:HG3	2.00	0.42
1:M:188:ARG:NH1	1:M:199:LYS:N	2.67	0.42
1:K:13:ALA:CB	1:K:117:PRO:HA	2.50	0.42
1:K:188:ARG:NH1	1:K:199:LYS:N	2.67	0.42
2:D:7:ASN:HB2	4:D:1654:HOH:O	2.19	0.42
2:L:250:LEU:CB	2:L:252:LEU:HG	2.50	0.42
2:P:241:GLY:O	2:P:243:VAL:HG23	2.19	0.42
2:N:192:ASN:HA	2:N:241:GLY:O	2.19	0.42
1:E:93:MET:HE1	1:E:98:LEU:HD23	2.01	0.42
1:C:155:LEU:HD12	1:C:187:TYR:HB3	2.01	0.42
2:N:122:ALA:N	2:N:153:ASP:OD1	2.53	0.42
1:A:117:PRO:O	1:A:120:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:113:SER:OG	2:L:81:SER:N	2.47	0.42
1:C:132:ARG:C	1:C:133:PHE:CD1	2.93	0.42
2:D:126:ILE:CD1	2:D:150:ALA:HB2	2.24	0.42
1:I:39:ASN:HD21	1:I:43:VAL:CG1	2.18	0.42
2:N:126:ILE:HD11	2:N:150:ALA:HB2	2.02	0.42
2:N:11:ILE:HA	2:N:12:PRO:HD2	1.89	0.42
2:J:20:VAL:CG1	2:J:22:VAL:HG13	2.50	0.42
1:M:134:ARG:HD2	1:M:141:THR:OG1	2.20	0.42
2:J:184:THR:HA	2:J:248:VAL:O	2.19	0.42
1:M:149:TYR:CG	1:M:169:PRO:HD3	2.54	0.42
2:B:116:GLY:HA2	2:B:189:LYS:CE	2.47	0.42
2:P:169:THR:OG1	2:P:181:ILE:HG23	2.19	0.42
2:J:30:VAL:HG12	2:J:31:GLY:N	2.34	0.42
2:L:1:PHE:CD1	2:L:133:GLN:HG3	2.55	0.42
1:I:28:ASN:O	1:I:29:SER:CB	2.68	0.42
1:M:31:TYR:O	1:M:56:ALA:HA	2.20	0.42
2:D:118:VAL:HG12	2:D:118:VAL:O	2.19	0.42
2:D:212:THR:O	2:D:269:GLN:HB2	2.20	0.42
1:M:177:LEU:HD12	1:M:178:PRO:CD	2.40	0.42
1:I:135:ARG:CZ	1:I:177:LEU:HD21	2.50	0.42
1:A:122:LEU:HD12	1:A:123:PRO:N	2.35	0.42
2:L:95:TYR:OH	2:L:103:TRP:CA	2.66	0.42
1:K:156:ASN:C	1:K:158:GLY:N	2.73	0.42
1:E:142:LEU:HD22	1:E:142:LEU:N	2.34	0.42
1:A:142:LEU:N	1:A:142:LEU:HD22	2.35	0.42
2:D:135:ASN:HD21	2:D:138:ASN:HD21	1.66	0.42
2:N:8:GLY:O	2:N:9:THR:C	2.57	0.42
1:A:67:ILE:N	1:A:67:ILE:HD12	2.34	0.42
1:I:50:VAL:HG12	1:I:51:THR:N	2.34	0.42
1:C:177:LEU:HA	1:C:178:PRO:HD2	1.87	0.42
2:D:201:THR:CB	2:D:206:ASN:ND2	2.83	0.42
2:F:212:THR:O	2:F:269:GLN:HB2	2.20	0.42
1:M:135:ARG:CZ	1:M:177:LEU:HD21	2.50	0.42
1:I:135:ARG:NH2	1:I:181:ALA:HB1	2.34	0.42
2:J:58:LEU:H	2:J:90:THR:HG21	1.79	0.42
2:F:136:ASN:H	2:F:136:ASN:ND2	2.17	0.42
2:P:222:GLY:C	2:P:257:ALA:HB3	2.40	0.42
2:P:184:THR:HA	2:P:248:VAL:O	2.19	0.42
2:L:48:TYR:HB2	2:L:52:ILE:CD1	2.48	0.42
1:C:122:LEU:C	1:C:122:LEU:HD12	2.38	0.42
1:I:122:LEU:CD1	1:I:126:GLN:HB3	2.50	0.42
2:L:30:VAL:HG12	2:L:31:GLY:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:117:PRO:O	1:O:119:LYS:N	2.53	0.42
1:I:117:PRO:O	1:I:119:LYS:N	2.53	0.42
1:I:188:ARG:NH1	1:I:199:LYS:H	2.18	0.42
1:K:57:MET:HA	1:K:61:LYS:HE3	2.00	0.42
2:J:13:ILE:HG23	3:J:1605:MAN:O2	2.20	0.42
1:A:107:ILE:HG12	4:A:213:HOH:O	2.19	0.42
1:I:41:ASP:C	1:I:43:VAL:H	2.22	0.42
2:N:41:GLN:C	2:N:42:ILE:HG13	2.40	0.42
2:L:58:LEU:H	2:L:90:THR:HG21	1.78	0.42
2:D:221:VAL:HG12	2:D:222:GLY:N	2.35	0.42
2:P:95:TYR:OH	2:P:103:TRP:CA	2.66	0.42
2:P:14:GLY:HA2	2:P:142:PHE:CZ	2.55	0.42
1:I:188:ARG:NH1	1:I:199:LYS:N	2.67	0.42
2:L:96:ASN:HD22	2:L:96:ASN:N	2.10	0.42
1:M:108:ILE:HB	2:N:275:THR:HG23	2.02	0.42
2:D:215:PHE:HD1	2:D:267:ASN:OD1	2.03	0.42
2:N:169:THR:OG1	2:N:181:ILE:HG23	2.20	0.42
1:O:77:GLN:HA	1:O:77:GLN:NE2	2.35	0.42
1:I:31:TYR:O	1:I:56:ALA:HA	2.20	0.42
2:J:207:SER:HB3	2:J:233:PRO:HB3	2.01	0.42
2:L:207:SER:HB3	2:L:233:PRO:HB3	2.01	0.42
2:L:223:VAL:CG1	2:L:224:GLN:N	2.82	0.42
1:A:94:ASP:OD1	2:B:168:VAL:HG11	2.20	0.42
1:O:136:SER:C	1:O:177:LEU:HD23	2.39	0.42
1:K:134:ARG:HD2	1:K:141:THR:OG1	2.20	0.42
1:C:94:ASP:OD1	2:D:168:VAL:HG11	2.20	0.42
1:O:142:LEU:HD22	1:O:142:LEU:N	2.35	0.42
1:O:149:TYR:CG	1:O:169:PRO:HD3	2.54	0.42
1:C:122:LEU:HD12	1:C:123:PRO:N	2.35	0.42
2:F:221:VAL:HG12	2:F:222:GLY:N	2.35	0.42
1:O:13:ALA:CB	1:O:117:PRO:HA	2.50	0.42
1:O:156:ASN:C	1:O:158:GLY:N	2.73	0.42
2:F:111:PRO:HB3	2:F:156:VAL:HG21	2.02	0.42
2:B:226:THR:HG22	2:B:255:ASN:HD21	1.84	0.41
1:A:71:THR:O	1:A:73:ASN:N	2.51	0.41
2:J:163:VAL:HA	2:J:185:VAL:CG2	2.36	0.41
1:E:132:ARG:C	1:E:133:PHE:CD1	2.93	0.41
2:N:184:THR:HA	2:N:248:VAL:O	2.20	0.41
2:D:90:THR:HG23	2:D:91:PRO:N	2.34	0.41
2:L:14:GLY:HA2	2:L:142:PHE:CZ	2.54	0.41
1:M:156:ASN:C	1:M:158:GLY:N	2.73	0.41
1:K:28:ASN:O	1:K:29:SER:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:142:LEU:N	1:C:142:LEU:HD22	2.34	0.41
2:J:136:ASN:HD22	2:J:136:ASN:N	2.18	0.41
2:F:38:LEU:C	2:F:40:THR:H	2.22	0.41
2:P:8:GLY:O	2:P:9:THR:C	2.57	0.41
2:L:122:ALA:N	2:L:153:ASP:OD1	2.53	0.41
2:L:64:TYR:CE1	2:L:128:VAL:HG23	2.55	0.41
1:C:67:ILE:HD12	1:C:67:ILE:N	2.34	0.41
1:I:77:GLN:HA	1:I:77:GLN:NE2	2.35	0.41
1:E:67:ILE:HD12	1:E:67:ILE:N	2.34	0.41
2:B:201:THR:CB	2:B:206:ASN:ND2	2.83	0.41
2:F:170:VAL:C	2:F:172:LEU:N	2.73	0.41
2:J:126:ILE:HD11	2:J:150:ALA:HB2	2.02	0.41
1:M:136:SER:C	1:M:177:LEU:HD23	2.40	0.41
1:I:134:ARG:HD2	1:I:141:THR:OG1	2.20	0.41
2:D:136:ASN:HD22	2:D:136:ASN:N	2.16	0.41
1:K:12:PRO:HD2	1:K:15:GLN:HG3	2.00	0.41
1:M:122:LEU:CD1	1:M:126:GLN:HB3	2.50	0.41
1:K:122:LEU:CD1	1:K:126:GLN:HB3	2.50	0.41
2:P:116:GLY:O	2:P:156:VAL:O	2.38	0.41
2:P:30:VAL:HG12	2:P:31:GLY:N	2.34	0.41
2:J:116:GLY:O	2:J:156:VAL:O	2.38	0.41
2:N:14:GLY:HA2	2:N:142:PHE:CZ	2.55	0.41
2:J:53:THR:H	2:J:136:ASN:HD21	1.68	0.41
2:J:140:ASP:OD1	3:J:1605:MAN:O3	2.31	0.41
1:E:117:PRO:O	1:E:120:LEU:HG	2.20	0.41
2:P:19:ASN:OD1	2:P:147:ASN:HB2	2.20	0.41
2:J:165:ALA:O	2:J:166:ARG:C	2.59	0.41
1:C:181:ALA:HB1	1:C:182:GLY:H	1.53	0.41
2:N:207:SER:HB3	2:N:233:PRO:HB3	2.01	0.41
2:D:201:THR:HB	2:D:206:ASN:ND2	2.36	0.41
1:I:135:ARG:HH12	1:I:177:LEU:HD11	1.82	0.41
1:I:179:SER:C	1:I:181:ALA:H	2.20	0.41
1:M:185:ILE:O	1:M:202:GLY:N	2.35	0.41
2:B:192:ASN:HA	2:B:241:GLY:O	2.20	0.41
1:E:12:PRO:CB	1:E:15:GLN:HG3	2.48	0.41
1:O:122:LEU:CD1	1:O:126:GLN:HB3	2.50	0.41
2:L:116:GLY:O	2:L:156:VAL:O	2.38	0.41
1:M:188:ARG:NH1	1:M:199:LYS:H	2.17	0.41
1:I:156:ASN:C	1:I:158:GLY:N	2.73	0.41
2:N:1:PHE:CD1	2:N:133:GLN:HG3	2.54	0.41
2:J:227:ARG:HG2	2:J:232:ILE:HD11	2.02	0.41
1:O:28:ASN:O	1:O:29:SER:CB	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:142:LEU:HD22	1:G:142:LEU:N	2.34	0.41
2:L:44:CYS:O	2:L:101:LYS:N	2.50	0.41
2:N:165:ALA:O	2:N:166:ARG:C	2.59	0.41
1:K:77:GLN:HA	1:K:77:GLN:NE2	2.35	0.41
2:F:126:ILE:CD1	2:F:150:ALA:HB2	2.25	0.41
2:B:170:VAL:C	2:B:172:LEU:N	2.74	0.41
1:O:135:ARG:CZ	1:O:177:LEU:HD21	2.50	0.41
1:K:135:ARG:CZ	1:K:177:LEU:HD21	2.50	0.41
2:D:136:ASN:H	2:D:136:ASN:ND2	2.17	0.41
1:G:186:THR:CG2	1:G:199:LYS:HZ2	2.33	0.41
2:J:19:ASN:OD1	2:J:147:ASN:HB2	2.20	0.41
1:C:38:GLU:OE1	1:C:110:ARG:NH2	2.46	0.41
1:I:13:ALA:CB	1:I:117:PRO:HA	2.50	0.41
2:P:227:ARG:HG2	2:P:232:ILE:HD11	2.03	0.41
2:J:250:LEU:CB	2:J:252:LEU:HG	2.50	0.41
2:P:53:THR:H	2:P:136:ASN:HD21	1.66	0.41
2:F:162:ASP:HB3	2:F:186:TYR:CZ	2.55	0.41
1:K:31:TYR:O	1:K:56:ALA:HA	2.19	0.41
2:L:197:LEU:CD1	2:L:225:LEU:HD12	2.43	0.41
2:L:227:ARG:HG2	2:L:232:ILE:HD11	2.03	0.41
2:F:201:THR:HB	2:F:206:ASN:ND2	2.35	0.41
1:O:39:ASN:HD21	1:O:43:VAL:CG1	2.18	0.41
1:I:140:LEU:C	1:I:140:LEU:HD23	2.41	0.41
2:L:184:THR:HA	2:L:248:VAL:O	2.20	0.41
1:K:117:PRO:O	1:K:119:LYS:N	2.53	0.41
1:K:188:ARG:NH1	1:K:199:LYS:H	2.18	0.41
1:O:108:ILE:HB	2:P:275:THR:HG23	2.03	0.41
2:L:169:THR:OG1	2:L:181:ILE:HG23	2.20	0.41
2:F:138:ASN:HD22	2:F:138:ASN:C	2.23	0.41
1:C:178:PRO:O	1:C:179:SER:HB3	2.20	0.41
1:K:140:LEU:C	1:K:140:LEU:HD23	2.41	0.41
2:H:136:ASN:ND2	2:H:136:ASN:H	2.18	0.41
2:L:222:GLY:C	2:L:257:ALA:HB3	2.41	0.41
2:J:29:ASN:OD1	2:J:157:PRO:HD2	2.20	0.41
1:M:80:GLU:HG3	1:M:148:TYR:HA	2.02	0.41
2:N:116:GLY:O	2:N:156:VAL:O	2.37	0.41
2:B:5:THR:HG22	2:B:9:THR:N	2.35	0.41
2:J:169:THR:OG1	2:J:181:ILE:HG23	2.20	0.41
2:P:44:CYS:O	2:P:101:LYS:N	2.51	0.41
1:K:99:THR:C	1:K:100:GLU:HG3	2.41	0.41
1:A:178:PRO:O	1:A:179:SER:HB3	2.21	0.41
1:M:135:ARG:HH12	1:M:177:LEU:HD11	1.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:22:VAL:HG12	2:N:41:GLN:HG3	2.02	0.41
2:N:20:VAL:CG1	2:N:22:VAL:HG13	2.50	0.41
1:O:140:LEU:HD23	1:O:140:LEU:C	2.41	0.41
2:L:20:VAL:CG1	2:L:22:VAL:HG13	2.50	0.41
2:N:90:THR:HG23	2:N:91:PRO:O	2.21	0.41
2:N:19:ASN:OD1	2:N:147:ASN:HB2	2.21	0.41
1:C:183:SER:C	1:C:185:ILE:N	2.74	0.41
2:N:227:ARG:HG2	2:N:232:ILE:HD11	2.03	0.41
2:P:67:VAL:CG2	2:P:126:ILE:HG23	2.36	0.41
1:I:133:PHE:HB3	1:I:134:ARG:H	1.70	0.41
1:E:94:ASP:OD1	2:F:168:VAL:HG11	2.20	0.41
1:G:183:SER:C	1:G:185:ILE:N	2.74	0.41
1:A:51:THR:HA	1:A:52:PRO:C	2.41	0.41
1:M:13:ALA:CB	1:M:117:PRO:HA	2.50	0.41
2:P:250:LEU:CB	2:P:252:LEU:HG	2.50	0.41
2:P:46:ASN:HD22	2:P:96:ASN:HA	1.85	0.41
2:B:207:SER:HB3	2:B:233:PRO:HB3	2.02	0.41
2:H:215:PHE:HD1	2:H:267:ASN:OD1	2.03	0.41
2:N:53:THR:H	2:N:136:ASN:HD21	1.67	0.41
2:B:215:PHE:HD1	2:B:267:ASN:OD1	2.04	0.41
1:I:24:ASN:HB2	1:I:57:MET:HE3	2.01	0.41
2:L:136:ASN:HD22	2:L:136:ASN:N	2.17	0.41
1:M:99:THR:C	1:M:100:GLU:HG3	2.41	0.41
2:D:1:PHE:CG	2:D:133:GLN:HG3	2.56	0.41
1:G:107:ILE:HG12	4:G:216:HOH:O	2.21	0.41
2:P:165:ALA:O	2:P:166:ARG:C	2.59	0.41
2:H:201:THR:CB	2:H:206:ASN:HD22	2.34	0.41
2:B:226:THR:CG2	2:B:255:ASN:HD21	2.33	0.41
1:G:140:LEU:CD2	1:G:140:LEU:C	2.89	0.41
1:G:71:THR:O	1:G:73:ASN:N	2.51	0.41
1:A:174:THR:O	1:A:174:THR:CG2	2.68	0.41
1:A:181:ALA:HB1	1:A:182:GLY:H	1.53	0.41
2:H:212:THR:O	2:H:269:GLN:HB2	2.20	0.41
2:N:67:VAL:HG21	2:N:126:ILE:CG2	2.36	0.41
1:O:135:ARG:HH12	1:O:177:LEU:HD11	1.83	0.41
2:P:20:VAL:CG1	2:P:22:VAL:HG13	2.51	0.41
2:J:20:VAL:CG2	2:J:42:ILE:HD11	2.50	0.41
1:M:133:PHE:HB3	1:M:134:ARG:H	1.71	0.41
2:F:168:VAL:HG22	2:F:168:VAL:O	2.21	0.41
2:F:92:ARG:NH1	2:F:92:ARG:CG	2.83	0.41
2:N:222:GLY:C	2:N:257:ALA:HB3	2.41	0.41
2:J:222:GLY:C	2:J:257:ALA:HB3	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:262:GLN:HE21	2:P:262:GLN:HA	1.86	0.41
2:L:262:GLN:HA	2:L:262:GLN:HE21	1.85	0.41
2:B:33:ASN:HA	2:B:33:ASN:HD22	1.60	0.41
2:N:262:GLN:HA	2:N:262:GLN:HE21	1.85	0.41
2:D:116:GLY:HA2	2:D:189:LYS:CE	2.47	0.41
1:K:126:GLN:O	1:K:126:GLN:HG2	2.21	0.41
1:M:13:ALA:HB3	1:M:118:ALA:H	1.84	0.41
1:M:117:PRO:O	1:M:119:LYS:N	2.53	0.41
1:E:198:PRO:O	1:E:200:MET:HG2	2.21	0.41
1:A:198:PRO:O	1:A:200:MET:HG2	2.21	0.41
2:N:136:ASN:HD22	2:N:136:ASN:N	2.18	0.41
2:N:64:TYR:CE1	2:N:128:VAL:HG23	2.56	0.41
1:A:129:GLU:H	1:A:129:GLU:HG3	1.51	0.41
1:M:140:LEU:HD23	1:M:140:LEU:C	2.41	0.41
1:M:142:LEU:HD22	1:M:142:LEU:N	2.35	0.41
1:K:80:GLU:HG3	1:K:148:TYR:HA	2.03	0.41
1:A:27:GLU:CG	1:A:60:LYS:HD2	2.49	0.41
1:E:167:VAL:HA	1:E:168:PRO:HD2	1.75	0.41
2:P:175:TYR:CZ	2:P:263:VAL:HB	2.56	0.41
2:D:5:THR:N	2:D:9:THR:O	2.51	0.41
1:C:198:PRO:O	1:C:200:MET:HG2	2.21	0.41
2:P:120:ILE:O	2:P:153:ASP:HA	2.21	0.41
2:F:135:ASN:HD21	2:F:138:ASN:HD21	1.67	0.41
2:L:165:ALA:O	2:L:166:ARG:C	2.59	0.41
1:G:80:GLU:HA	1:G:115:TYR:O	2.21	0.41
1:I:99:THR:C	1:I:100:GLU:HG3	2.41	0.41
2:N:202:ALA:HB2	2:N:210:THR:CG2	2.34	0.40
1:I:142:LEU:HD22	1:I:142:LEU:N	2.36	0.40
1:O:185:ILE:O	1:O:202:GLY:N	2.35	0.40
1:G:188:ARG:HG2	1:G:199:LYS:HA	2.04	0.40
2:P:52:ILE:HD12	3:P:1607:MAN:H61	2.04	0.40
2:F:90:THR:HG23	2:F:91:PRO:N	2.35	0.40
1:O:182:GLY:O	1:O:183:SER:CB	2.65	0.40
1:M:126:GLN:O	1:M:126:GLN:HG2	2.21	0.40
1:C:168:PRO:HA	1:C:169:PRO:HD3	1.87	0.40
2:L:175:TYR:CZ	2:L:263:VAL:HB	2.57	0.40
2:N:46:ASN:HD22	2:N:96:ASN:HA	1.86	0.40
2:D:138:ASN:C	2:D:138:ASN:HD22	2.24	0.40
2:N:128:VAL:HG12	2:N:128:VAL:O	2.21	0.40
2:L:19:ASN:OD1	2:L:147:ASN:HB2	2.21	0.40
2:H:162:ASP:HB3	2:H:186:TYR:CZ	2.56	0.40
2:H:170:VAL:C	2:H:172:LEU:N	2.74	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:168:VAL:HG22	2:H:168:VAL:O	2.22	0.40
2:D:168:VAL:HG22	2:D:168:VAL:O	2.20	0.40
2:D:59:GLN:HG2	2:D:132:ARG:CD	2.43	0.40
2:L:41:GLN:C	2:L:42:ILE:HG13	2.40	0.40
1:G:51:THR:HA	1:G:52:PRO:C	2.41	0.40
1:M:101:ASN:ND2	2:N:268:VAL:N	2.69	0.40
1:I:80:GLU:HG3	1:I:148:TYR:HA	2.03	0.40
2:B:90:THR:HG23	2:B:91:PRO:N	2.36	0.40
2:N:175:TYR:CZ	2:N:263:VAL:HB	2.56	0.40
1:C:191:ASN:ND2	1:C:195:ALA:HB3	2.34	0.40
1:G:198:PRO:O	1:G:200:MET:HG2	2.21	0.40
2:D:111:PRO:HB3	2:D:156:VAL:HG21	2.02	0.40
2:B:138:ASN:HD22	2:B:138:ASN:C	2.24	0.40
1:I:108:ILE:HB	2:J:275:THR:HG23	2.02	0.40
1:O:99:THR:C	1:O:100:GLU:HG3	2.42	0.40
2:H:228:ASN:HD22	2:H:228:ASN:N	2.19	0.40
1:C:188:ARG:HG2	1:C:199:LYS:HA	2.03	0.40
2:D:218:ALA:HB2	2:D:266:GLY:CA	2.51	0.40
1:O:193:TYR:HB3	2:P:157:PRO:HG3	2.03	0.40
1:A:167:VAL:HA	1:A:168:PRO:HD2	1.76	0.40
1:G:167:VAL:HA	1:G:168:PRO:HD2	1.76	0.40
1:A:82:LEU:HD12	1:A:83:PHE:H	1.84	0.40
2:P:128:VAL:HG12	2:P:128:VAL:O	2.21	0.40
2:N:223:VAL:CG1	2:N:224:GLN:N	2.83	0.40
1:G:178:PRO:O	1:G:179:SER:HB3	2.21	0.40
1:A:155:LEU:HA	1:A:186:THR:O	2.22	0.40
2:N:24:LEU:O	2:N:152:ASN:ND2	2.51	0.40
1:E:155:LEU:HA	1:E:186:THR:O	2.22	0.40
1:K:142:LEU:N	1:K:142:LEU:HD22	2.36	0.40
2:P:11:ILE:HA	2:P:12:PRO:HD2	1.89	0.40
2:J:22:VAL:HG12	2:J:41:GLN:HG3	2.03	0.40
2:B:136:ASN:HD22	2:B:136:ASN:N	2.18	0.40
1:K:8:ARG:NH1	1:K:190:ILE:CG2	2.85	0.40
1:O:103:LEU:HD23	2:P:181:ILE:HD11	2.03	0.40
1:G:191:ASN:O	1:G:194:GLY:N	2.46	0.40
2:J:46:ASN:HD22	2:J:96:ASN:HA	1.86	0.40
2:L:128:VAL:O	2:L:128:VAL:HG12	2.21	0.40
2:L:64:TYR:N	2:L:64:TYR:CD1	2.89	0.40
2:P:106:ALA:CB	2:P:108:TYR:HE1	2.35	0.40
2:H:1:PHE:CG	2:H:133:GLN:HG3	2.57	0.40
1:E:129:GLU:HG3	1:E:129:GLU:H	1.52	0.40
2:N:231:ILE:CG2	2:N:232:ILE:N	2.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:231:ILE:CG2	2:L:232:ILE:N	2.84	0.40
2:N:209:PHE:CE2	2:N:272:ILE:HG23	2.57	0.40
1:E:47:ARG:NH2	1:E:74:GLN:NE2	2.55	0.40
1:A:140:LEU:C	1:A:140:LEU:CD2	2.90	0.40
2:P:162:ASP:O	2:P:185:VAL:HA	2.22	0.40
2:P:22:VAL:HG12	2:P:41:GLN:HG3	2.03	0.40
2:L:22:VAL:HG12	2:L:41:GLN:HG3	2.02	0.40
2:L:90:THR:HG23	2:L:91:PRO:O	2.22	0.40
1:O:101:ASN:ND2	2:P:268:VAL:N	2.69	0.40
1:M:193:TYR:HB3	2:N:157:PRO:HG3	2.04	0.40
2:B:262:GLN:CA	2:B:262:GLN:HE21	2.25	0.40
1:I:78:ASP:O	1:I:170:MET:HE1	2.20	0.40
2:F:116:GLY:HA2	2:F:189:LYS:CE	2.47	0.40
1:O:126:GLN:O	1:O:126:GLN:HG2	2.21	0.40
2:J:120:ILE:O	2:J:153:ASP:HA	2.21	0.40
2:B:118:VAL:HG12	2:B:118:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	3	8
1	C	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	3	8
1	E	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	3	8
1	G	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	3	8
1	I	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	6
1	K	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	6
1	M	203/205 (99%)	162 (80%)	29 (14%)	12 (6%)	2	6
1	O	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	2	6
2	B	277/279 (99%)	244 (88%)	24 (9%)	9 (3%)	6	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	5	17
2	F	277/279 (99%)	244 (88%)	23 (8%)	10 (4%)	5	17
2	H	277/279 (99%)	243 (88%)	24 (9%)	10 (4%)	5	17
2	J	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	3
2	L	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	3
2	N	277/279 (99%)	195 (70%)	60 (22%)	22 (8%)	1	3
2	P	277/279 (99%)	196 (71%)	59 (21%)	22 (8%)	1	3
All	All	3840/3872 (99%)	3058 (80%)	563 (15%)	219 (6%)	3	7

All (219) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	119	LYS
1	A	181	ALA
1	A	183	SER
2	B	175	TYR
2	B	218	ALA
1	C	29	SER
1	C	119	LYS
1	C	181	ALA
1	C	183	SER
2	D	175	TYR
2	D	218	ALA
1	E	29	SER
1	E	119	LYS
1	E	181	ALA
1	E	183	SER
2	F	175	TYR
2	F	218	ALA
1	G	29	SER
1	G	119	LYS
1	G	181	ALA
1	G	183	SER
2	H	175	TYR
2	H	218	ALA
1	I	29	SER
1	I	119	LYS
1	I	181	ALA
1	I	183	SER

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Mol	Chain	Res	Type
1	K	29	SER
1	K	119	LYS
1	K	181	ALA
1	K	183	SER
2	L	264	THR
1	M	29	SER
1	M	119	LYS
1	M	181	ALA
1	M	183	SER
2	N	264	THR
1	O	29	SER
1	O	119	LYS
1	O	181	ALA
1	O	183	SER
2	P	264	THR
1	A	26	ASP
1	A	192	ASP
2	B	116	GLY
2	B	167	ASP
2	B	173	PRO
2	B	174	ASP
2	B	215	PHE
2	B	221	VAL
1	C	26	ASP
1	C	192	ASP
2	D	116	GLY
2	D	167	ASP
2	D	173	PRO
2	D	174	ASP
2	D	215	PHE
2	D	221	VAL
1	E	26	ASP
1	E	192	ASP
2	F	116	GLY
2	F	167	ASP
2	F	173	PRO
2	F	174	ASP
2	F	215	PHE
2	F	221	VAL
1	G	26	ASP
1	G	192	ASP
2	H	116	GLY

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Mol	Chain	Res	Type
2	H	167	ASP
2	H	173	PRO
2	H	174	ASP
2	H	215	PHE
2	H	221	VAL
1	I	62	GLU
2	J	9	THR
2	J	22	VAL
2	J	32	GLN
2	J	116	GLY
2	J	157	PRO
2	J	168	VAL
2	J	190	SER
2	J	247	ALA
2	J	264	THR
1	K	62	GLU
2	L	9	THR
2	L	22	VAL
2	L	32	GLN
2	L	116	GLY
2	L	157	PRO
2	L	168	VAL
2	L	190	SER
2	L	247	ALA
1	M	62	GLU
2	N	9	THR
2	N	22	VAL
2	N	116	GLY
2	N	157	PRO
2	N	168	VAL
2	N	190	SER
2	N	247	ALA
1	O	62	GLU
2	P	9	THR
2	P	22	VAL
2	P	32	GLN
2	P	116	GLY
2	P	157	PRO
2	P	168	VAL
2	P	190	SER
2	P	247	ALA
1	A	134	ARG

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Mol	Chain	Res	Type
1	A	138	ASN
1	C	134	ARG
1	C	138	ASN
1	E	134	ARG
1	E	138	ASN
1	G	134	ARG
1	G	138	ASN
1	I	26	ASP
2	J	97	SER
2	J	173	PRO
2	J	206	ASN
2	J	235	ASN
2	J	242	ALA
1	K	26	ASP
2	L	97	SER
2	L	173	PRO
2	L	206	ASN
2	L	235	ASN
2	L	242	ALA
1	M	26	ASP
2	N	32	GLN
2	N	97	SER
2	N	173	PRO
2	N	206	ASN
2	N	235	ASN
2	N	242	ALA
1	O	26	ASP
2	P	97	SER
2	P	173	PRO
2	P	206	ASN
2	P	235	ASN
2	P	242	ALA
1	A	72	ASN
1	A	91	PRO
1	C	72	ASN
1	C	91	PRO
1	E	72	ASN
1	G	72	ASN
1	G	91	PRO
1	I	91	PRO
1	I	121	ALA
1	I	134	ARG

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Mol	Chain	Res	Type
1	I	138	ASN
2	J	166	ARG
2	J	261	GLY
1	K	91	PRO
1	K	121	ALA
1	K	134	ARG
1	K	138	ASN
2	L	166	ARG
2	L	261	GLY
1	M	91	PRO
1	M	121	ALA
1	M	134	ARG
1	M	138	ASN
2	N	166	ARG
2	N	261	GLY
1	O	91	PRO
1	O	121	ALA
1	O	134	ARG
1	O	138	ASN
2	P	166	ARG
2	P	261	GLY
1	E	91	PRO
1	I	164	ASN
2	J	40	THR
2	J	100	ASP
1	K	164	ASN
2	L	40	THR
2	L	100	ASP
1	M	164	ASN
2	N	40	THR
2	N	100	ASP
2	N	217	PRO
1	O	164	ASN
2	P	40	THR
2	P	100	ASP
1	A	147	PRO
1	C	147	PRO
2	D	260	GLY
1	E	147	PRO
2	F	260	GLY
1	G	147	PRO
2	H	260	GLY

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Mol	Chain	Res	Type
2	J	217	PRO
2	L	217	PRO
2	P	217	PRO
2	B	260	GLY
2	J	26	PRO
1	I	42	GLY
2	J	273	GLY
2	J	274	VAL
1	K	42	GLY
2	L	26	PRO
2	L	273	GLY
2	L	274	VAL
1	M	42	GLY
2	N	26	PRO
2	N	273	GLY
1	O	42	GLY
2	P	26	PRO
2	P	273	GLY
2	P	274	VAL
2	N	274	VAL
2	D	104	PRO
2	F	104	PRO
2	H	104	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	160 (91%)	16 (9%)	14	37
1	C	176/176 (100%)	159 (90%)	17 (10%)	12	32
1	E	176/176 (100%)	160 (91%)	16 (9%)	14	37
1	G	176/176 (100%)	160 (91%)	16 (9%)	14	37
1	I	176/176 (100%)	165 (94%)	11 (6%)	25	59
1	K	176/176 (100%)	164 (93%)	12 (7%)	22	54
1	M	176/176 (100%)	165 (94%)	11 (6%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	176/176 (100%)	165 (94%)	11 (6%)	25	59
2	B	226/226 (100%)	208 (92%)	18 (8%)	17	44
2	D	226/226 (100%)	208 (92%)	18 (8%)	17	44
2	F	226/226 (100%)	207 (92%)	19 (8%)	16	41
2	H	226/226 (100%)	207 (92%)	19 (8%)	16	41
2	J	226/226 (100%)	214 (95%)	12 (5%)	32	67
2	L	226/226 (100%)	214 (95%)	12 (5%)	32	67
2	N	226/226 (100%)	214 (95%)	12 (5%)	32	67
2	P	226/226 (100%)	213 (94%)	13 (6%)	28	63
All	All	3216/3216 (100%)	2983 (93%)	233 (7%)	21	50

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	23	THR
1	A	28	ASN
1	A	44	LYS
1	A	47	ARG
1	A	61	LYS
1	A	62	GLU
1	A	104	GLN
1	A	129	GLU
1	A	135	ARG
1	A	142	LEU
1	A	143	ILE
1	A	146	THR
1	A	173	SER
1	A	200	MET
1	A	205	GLU
2	B	4	LYS
2	B	5	THR
2	B	33	ASN
2	B	40	THR
2	B	57	THR
2	B	59	GLN
2	B	81	SER
2	B	90	THR
2	B	96	ASN

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	126	ILE
2	B	136	ASN
2	B	138	ASN
2	B	190	SER
2	B	201	THR
2	B	211	ASN
2	B	262	GLN
2	B	271	ILE
1	C	8	ARG
1	C	23	THR
1	C	28	ASN
1	C	44	LYS
1	C	47	ARG
1	C	61	LYS
1	C	62	GLU
1	C	104	GLN
1	C	129	GLU
1	C	135	ARG
1	C	142	LEU
1	C	143	ILE
1	C	146	THR
1	C	173	SER
1	C	174	THR
1	C	200	MET
1	C	205	GLU
2	D	4	LYS
2	D	5	THR
2	D	33	ASN
2	D	40	THR
2	D	57	THR
2	D	59	GLN
2	D	81	SER
2	D	90	THR
2	D	96	ASN
2	D	107	LEU
2	D	126	ILE
2	D	136	ASN
2	D	138	ASN
2	D	190	SER
2	D	201	THR
2	D	211	ASN

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Mol	Chain	Res	Type
2	D	262	GLN
2	D	271	ILE
1	E	8	ARG
1	E	23	THR
1	E	28	ASN
1	E	44	LYS
1	E	47	ARG
1	E	61	LYS
1	E	62	GLU
1	E	104	GLN
1	E	129	GLU
1	E	135	ARG
1	E	142	LEU
1	E	143	ILE
1	E	146	THR
1	E	173	SER
1	E	200	MET
1	E	205	GLU
2	F	4	LYS
2	F	5	THR
2	F	33	ASN
2	F	40	THR
2	F	57	THR
2	F	59	GLN
2	F	81	SER
2	F	90	THR
2	F	96	ASN
2	F	107	LEU
2	F	126	ILE
2	F	136	ASN
2	F	138	ASN
2	F	190	SER
2	F	201	THR
2	F	211	ASN
2	F	226	THR
2	F	262	GLN
2	F	271	ILE
1	G	8	ARG
1	G	23	THR
1	G	28	ASN
1	G	44	LYS
1	G	47	ARG

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Mol	Chain	Res	Type
1	G	61	LYS
1	G	62	GLU
1	G	104	GLN
1	G	129	GLU
1	G	135	ARG
1	G	142	LEU
1	G	143	ILE
1	G	146	THR
1	G	173	SER
1	G	200	MET
1	G	205	GLU
2	H	4	LYS
2	H	5	THR
2	H	33	ASN
2	H	40	THR
2	H	57	THR
2	H	59	GLN
2	H	81	SER
2	H	90	THR
2	H	96	ASN
2	H	107	LEU
2	H	126	ILE
2	H	136	ASN
2	H	138	ASN
2	H	190	SER
2	H	201	THR
2	H	211	ASN
2	H	226	THR
2	H	262	GLN
2	H	271	ILE
1	I	8	ARG
1	I	28	ASN
1	I	43	VAL
1	I	44	LYS
1	I	47	ARG
1	I	62	GLU
1	I	85	MET
1	I	92	SER
1	I	135	ARG
1	I	183	SER
1	I	200	MET
2	J	33	ASN

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Mol	Chain	Res	Type
2	J	43	PHE
2	J	57	THR
2	J	96	ASN
2	J	103	TRP
2	J	121	LYS
2	J	136	ASN
2	J	157	PRO
2	J	183	LEU
2	J	184	THR
2	J	211	ASN
2	J	215	PHE
1	K	8	ARG
1	K	28	ASN
1	K	43	VAL
1	K	44	LYS
1	K	47	ARG
1	K	62	GLU
1	K	85	MET
1	K	92	SER
1	K	135	ARG
1	K	176	LYS
1	K	183	SER
1	K	200	MET
2	L	33	ASN
2	L	43	PHE
2	L	57	THR
2	L	96	ASN
2	L	103	TRP
2	L	121	LYS
2	L	136	ASN
2	L	157	PRO
2	L	183	LEU
2	L	184	THR
2	L	211	ASN
2	L	215	PHE
1	M	8	ARG
1	M	28	ASN
1	M	43	VAL
1	M	44	LYS
1	M	47	ARG
1	M	62	GLU
1	M	85	MET

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Mol	Chain	Res	Type
1	M	92	SER
1	M	135	ARG
1	M	183	SER
1	M	200	MET
2	N	33	ASN
2	N	43	PHE
2	N	57	THR
2	N	96	ASN
2	N	103	TRP
2	N	121	LYS
2	N	136	ASN
2	N	157	PRO
2	N	183	LEU
2	N	184	THR
2	N	211	ASN
2	N	215	PHE
1	O	8	ARG
1	O	28	ASN
1	O	43	VAL
1	O	44	LYS
1	O	47	ARG
1	O	62	GLU
1	O	85	MET
1	O	92	SER
1	O	135	ARG
1	O	183	SER
1	O	200	MET
2	P	33	ASN
2	P	37	ASP
2	P	43	PHE
2	P	57	THR
2	P	96	ASN
2	P	103	TRP
2	P	121	LYS
2	P	136	ASN
2	P	157	PRO
2	P	183	LEU
2	P	184	THR
2	P	211	ASN
2	P	215	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	28	ASN
1	A	72	ASN
1	A	74	GLN
1	A	86	ASN
1	A	126	GLN
1	A	184	ASN
2	B	32	GLN
2	B	33	ASN
2	B	41	GLN
2	B	70	ASN
2	B	136	ASN
2	B	138	ASN
2	B	206	ASN
2	B	211	ASN
2	B	219	GLN
2	B	224	GLN
2	B	228	ASN
2	B	255	ASN
2	B	262	GLN
2	B	279	GLN
1	C	15	GLN
1	C	28	ASN
1	C	72	ASN
1	C	74	GLN
1	C	86	ASN
1	C	126	GLN
1	C	184	ASN
2	D	23	ASN
2	D	32	GLN
2	D	33	ASN
2	D	41	GLN
2	D	136	ASN
2	D	138	ASN
2	D	206	ASN
2	D	211	ASN
2	D	219	GLN
2	D	224	GLN
2	D	228	ASN
2	D	255	ASN
2	D	262	GLN
2	D	279	GLN
1	E	15	GLN

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Mol	Chain	Res	Type
1	E	28	ASN
1	E	72	ASN
1	E	74	GLN
1	E	86	ASN
1	E	126	GLN
1	E	184	ASN
2	F	23	ASN
2	F	32	GLN
2	F	33	ASN
2	F	41	GLN
2	F	70	ASN
2	F	136	ASN
2	F	138	ASN
2	F	206	ASN
2	F	211	ASN
2	F	219	GLN
2	F	228	ASN
2	F	255	ASN
2	F	262	GLN
2	F	279	GLN
1	G	15	GLN
1	G	28	ASN
1	G	72	ASN
1	G	74	GLN
1	G	77	GLN
1	G	86	ASN
1	G	126	GLN
1	G	184	ASN
2	H	32	GLN
2	H	33	ASN
2	H	41	GLN
2	H	136	ASN
2	H	138	ASN
2	H	206	ASN
2	H	211	ASN
2	H	219	GLN
2	H	224	GLN
2	H	228	ASN
2	H	255	ASN
2	H	262	GLN
2	H	279	GLN
1	I	28	ASN

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Mol	Chain	Res	Type
1	I	72	ASN
1	I	74	GLN
1	I	77	GLN
1	I	86	ASN
1	I	101	ASN
1	I	104	GLN
1	I	126	GLN
1	I	184	ASN
2	J	19	ASN
2	J	33	ASN
2	J	70	ASN
2	J	96	ASN
2	J	136	ASN
2	J	138	ASN
2	J	151	ASN
2	J	191	GLN
2	J	211	ASN
2	J	224	GLN
2	J	228	ASN
2	J	255	ASN
2	J	262	GLN
2	J	269	GLN
2	J	279	GLN
1	K	28	ASN
1	K	72	ASN
1	K	74	GLN
1	K	77	GLN
1	K	86	ASN
1	K	101	ASN
1	K	104	GLN
1	K	126	GLN
1	K	184	ASN
2	L	33	ASN
2	L	70	ASN
2	L	96	ASN
2	L	136	ASN
2	L	138	ASN
2	L	143	GLN
2	L	151	ASN
2	L	191	GLN
2	L	211	ASN
2	L	219	GLN

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Mol	Chain	Res	Type
2	L	224	GLN
2	L	228	ASN
2	L	255	ASN
2	L	262	GLN
2	L	269	GLN
2	L	279	GLN
1	M	28	ASN
1	M	72	ASN
1	M	74	GLN
1	M	77	GLN
1	M	86	ASN
1	M	101	ASN
1	M	104	GLN
1	M	126	GLN
1	M	184	ASN
2	N	19	ASN
2	N	33	ASN
2	N	70	ASN
2	N	96	ASN
2	N	136	ASN
2	N	138	ASN
2	N	151	ASN
2	N	191	GLN
2	N	211	ASN
2	N	224	GLN
2	N	228	ASN
2	N	255	ASN
2	N	262	GLN
2	N	269	GLN
2	N	279	GLN
1	O	28	ASN
1	O	72	ASN
1	O	74	GLN
1	O	77	GLN
1	O	86	ASN
1	O	101	ASN
1	O	104	GLN
1	O	126	GLN
1	O	184	ASN
2	P	33	ASN
2	P	70	ASN
2	P	96	ASN

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Mol	Chain	Res	Type
2	P	136	ASN
2	P	138	ASN
2	P	151	ASN
2	P	191	GLN
2	P	211	ASN
2	P	219	GLN
2	P	224	GLN
2	P	228	ASN
2	P	255	ASN
2	P	262	GLN
2	P	269	GLN
2	P	279	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MAN	B	1500	-	12,12,12	0.38	0	17,17,17	0.40	0
3	MAN	D	1601	-	12,12,12	0.34	0	17,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	1502	-	12,12,12	0.41	0	17,17,17	0.61	0
3	MAN	H	1603	-	12,12,12	0.42	0	17,17,17	0.53	0
3	MAN	J	1605	-	12,12,12	0.26	0	17,17,17	0.36	0
3	MAN	L	1504	-	12,12,12	0.27	0	17,17,17	0.44	0
3	MAN	N	1506	-	12,12,12	0.22	0	17,17,17	0.44	0
3	MAN	P	1607	-	12,12,12	0.26	0	17,17,17	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	1500	-	-	0/2/22/22	0/1/1/1
3	MAN	D	1601	-	-	0/2/22/22	0/1/1/1
3	MAN	F	1502	-	-	0/2/22/22	0/1/1/1
3	MAN	H	1603	-	-	0/2/22/22	0/1/1/1
3	MAN	J	1605	-	-	0/2/22/22	0/1/1/1
3	MAN	L	1504	-	-	0/2/22/22	0/1/1/1
3	MAN	N	1506	-	-	0/2/22/22	0/1/1/1
3	MAN	P	1607	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	205/205 (100%)	0.56	11 (5%)	25	25	20, 55, 108, 132	0
1	C	205/205 (100%)	0.54	12 (5%)	22	21	20, 57, 108, 130	0
1	E	205/205 (100%)	0.47	7 (3%)	43	44	20, 59, 108, 129	0
1	G	205/205 (100%)	0.53	18 (8%)	10	8	19, 58, 110, 132	0
1	I	205/205 (100%)	4.03	147 (71%)	0	0	20, 168, 190, 196	0
1	K	205/205 (100%)	4.85	173 (84%)	0	0	20, 171, 195, 198	0
1	M	205/205 (100%)	4.68	174 (84%)	0	0	20, 170, 193, 198	0
1	O	205/205 (100%)	4.06	154 (75%)	0	0	20, 168, 193, 198	0
2	B	279/279 (100%)	0.35	7 (2%)	54	55	17, 40, 79, 114	0
2	D	279/279 (100%)	0.36	7 (2%)	54	55	18, 41, 80, 116	0
2	F	279/279 (100%)	0.28	4 (1%)	72	72	18, 41, 83, 112	0
2	H	279/279 (100%)	0.34	6 (2%)	59	60	17, 42, 83, 114	0
2	J	279/279 (100%)	2.12	109 (39%)	1	0	51, 112, 192, 200	0
2	L	279/279 (100%)	2.48	128 (45%)	1	0	56, 113, 190, 200	0
2	N	279/279 (100%)	2.68	148 (53%)	0	0	53, 115, 193, 200	0
2	P	279/279 (100%)	2.24	108 (38%)	1	0	50, 112, 191, 200	0
All	All	3872/3872 (100%)	1.82	1213 (31%)	1	1	17, 85, 186, 200	0

All (1213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	48	PHE	18.6
1	I	102	THR	17.3
2	L	270	SER	16.8
1	M	102	THR	15.4
1	K	95	LYS	15.2

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Mol	Chain	Res	Type	RSRZ
1	M	183	SER	14.9
1	M	150	LEU	14.8
1	K	102	THR	14.5
1	K	65	LEU	13.9
1	K	205	GLU	13.9
1	K	101	ASN	13.2
1	O	162	LEU	13.1
1	K	69	ASP	13.0
1	O	103	LEU	12.9
2	L	202	ALA	12.9
1	M	95	LYS	12.8
2	P	218	ALA	12.7
2	J	256	TYR	12.7
1	O	48	PHE	12.5
1	K	98	LEU	12.4
1	M	133	PHE	12.3
1	I	95	LYS	12.3
1	K	127	ALA	12.2
1	M	71	THR	12.2
1	I	127	ALA	12.2
1	I	205	GLU	12.2
1	K	104	GLN	12.1
2	N	179	VAL	12.1
1	M	179	SER	12.1
1	O	67	ILE	12.0
1	M	93	MET	11.9
1	K	170	MET	11.8
1	O	105	LEU	11.8
1	K	174	THR	11.7
1	M	18	VAL	11.7
1	O	71	THR	11.7
2	P	256	TYR	11.6
2	L	271	ILE	11.6
1	I	174	THR	11.3
1	K	18	VAL	11.2
1	K	184	ASN	11.1
1	K	48	PHE	11.1
2	P	215	PHE	11.0
1	M	184	ASN	11.0
2	J	217	PRO	11.0
1	M	105	LEU	10.9
2	P	214	SER	10.8

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Mol	Chain	Res	Type	RSRZ
1	O	95	LYS	10.7
1	K	135	ARG	10.7
1	K	150	LEU	10.7
1	M	162	LEU	10.7
2	P	217	PRO	10.6
1	M	104	GLN	10.5
2	N	168	VAL	10.5
1	K	183	SER	10.5
1	M	65	LEU	10.3
1	M	55	PHE	10.3
1	O	184	ASN	10.3
1	O	96	SER	10.2
2	J	268	VAL	10.2
2	J	215	PHE	9.9
1	M	205	GLU	9.9
1	K	93	MET	9.9
2	L	168	VAL	9.9
2	N	271	ILE	9.7
2	L	256	TYR	9.7
1	O	201	THR	9.6
1	M	201	THR	9.6
1	O	104	GLN	9.6
1	M	174	THR	9.5
2	N	218	ALA	9.4
2	P	272	ILE	9.4
2	N	181	ILE	9.4
1	I	67	ILE	9.3
1	I	184	ASN	9.3
2	P	202	ALA	9.3
1	I	65	LEU	9.3
1	I	133	PHE	9.2
1	K	71	THR	9.2
2	N	267	ASN	9.2
1	I	94	ASP	9.2
1	K	137	ALA	9.2
2	P	263	VAL	9.1
1	K	133	PHE	9.1
1	K	67	ILE	9.1
2	J	204	ALA	9.0
1	K	128	ALA	9.0
1	I	69	ASP	9.0
1	M	101	ASN	8.9

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Mol	Chain	Res	Type	RSRZ
2	J	213	ALA	8.9
1	K	94	ASP	8.9
1	I	150	LEU	8.8
2	L	223	VAL	8.8
2	L	116	GLY	8.8
1	O	150	LEU	8.8
1	K	103	LEU	8.8
1	M	135	ARG	8.7
1	M	47	ARG	8.7
1	K	34	GLN	8.7
1	I	135	ARG	8.7
2	P	179	VAL	8.7
1	K	201	THR	8.7
2	N	175	TYR	8.7
1	M	98	LEU	8.6
1	O	65	LEU	8.6
1	K	106	ALA	8.6
1	K	185	ILE	8.6
1	K	55	PHE	8.6
1	I	170	MET	8.6
1	K	157	ALA	8.6
2	N	214	SER	8.5
1	I	101	ASN	8.5
2	L	268	VAL	8.5
1	M	185	ILE	8.5
1	M	116	ARG	8.5
1	O	69	ASP	8.5
1	I	131	LEU	8.4
1	I	48	PHE	8.4
2	N	174	ASP	8.4
1	O	183	SER	8.4
2	J	179	VAL	8.3
1	O	94	ASP	8.3
1	O	102	THR	8.3
2	P	271	ILE	8.3
2	N	272	ILE	8.3
2	P	261	GLY	8.2
2	N	211	ASN	8.2
2	N	261	GLY	8.2
1	I	128	ALA	8.2
2	N	268	VAL	8.2
2	P	211	ASN	8.1

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Mol	Chain	Res	Type	RSRZ
1	K	19	GLN	8.1
2	N	207	SER	8.1
1	K	20	LEU	8.1
1	O	174	THR	8.1
1	M	155	LEU	8.1
1	O	177	LEU	8.0
2	N	260	GLY	8.0
2	N	270	SER	8.0
1	I	93	MET	7.9
1	I	20	LEU	7.9
1	K	162	LEU	7.9
2	N	172	LEU	7.9
1	K	200	MET	7.9
1	M	128	ALA	7.9
1	I	186	THR	7.9
2	J	212	THR	7.9
1	O	136	SER	7.8
1	I	35	SER	7.8
1	I	98	LEU	7.8
1	M	70	ALA	7.8
1	I	183	SER	7.8
1	M	148	TYR	7.8
1	M	151	THR	7.8
2	N	219	GLN	7.8
2	P	270	SER	7.7
1	M	67	ILE	7.7
1	O	20	LEU	7.7
1	O	18	VAL	7.7
1	K	105	LEU	7.7
1	I	162	LEU	7.7
1	O	205	GLU	7.6
2	N	202	ALA	7.6
1	I	157	ALA	7.6
2	P	216	SER	7.6
1	M	137	ALA	7.6
1	O	55	PHE	7.6
1	M	152	VAL	7.5
1	K	68	LEU	7.5
1	M	94	ASP	7.5
1	M	127	ALA	7.5
1	K	37	VAL	7.5
1	M	87	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
1	O	127	ALA	7.4
2	J	257	ALA	7.4
1	M	100	GLU	7.4
2	P	212	THR	7.4
1	K	173	SER	7.4
1	K	138	ASN	7.4
1	O	135	ARG	7.3
1	M	203	VAL	7.3
1	I	201	THR	7.3
2	N	256	TYR	7.3
2	L	181	ILE	7.3
2	L	182	PRO	7.3
1	I	4	LEU	7.3
2	J	271	ILE	7.3
2	L	222	GLY	7.3
1	O	98	LEU	7.2
1	M	11	TYR	7.2
1	O	87	VAL	7.2
2	N	222	GLY	7.2
2	J	175	TYR	7.2
1	K	36	TRP	7.2
1	O	133	PHE	7.2
1	K	96	SER	7.1
2	J	225	LEU	7.1
1	O	91	PRO	7.1
1	M	178	PRO	7.1
2	P	268	VAL	7.1
1	O	84	TRP	7.0
2	L	272	ILE	7.0
2	N	266	GLY	7.0
1	I	83	PHE	7.0
1	I	142	LEU	7.0
1	M	91	PRO	7.0
1	I	33	ILE	7.0
2	J	218	ALA	7.0
2	J	223	VAL	6.9
1	M	12	PRO	6.9
1	I	104	GLN	6.9
1	K	35	SER	6.9
1	O	35	SER	6.9
1	I	151	THR	6.9
2	P	213	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	K	9	VAL	6.8
2	N	215	PHE	6.8
1	M	52	PRO	6.8
1	O	128	ALA	6.8
1	I	18	VAL	6.8
2	N	20	VAL	6.8
2	P	222	GLY	6.7
1	K	4	LEU	6.7
1	I	55	PHE	6.7
1	O	52	PRO	6.7
1	M	69	ASP	6.7
2	L	232	ILE	6.7
1	K	92	SER	6.6
2	J	202	ALA	6.6
1	I	7	THR	6.6
1	O	7	THR	6.6
1	O	50	VAL	6.6
1	I	117	PRO	6.6
1	K	83	PHE	6.6
2	L	219	GLN	6.6
1	I	148	TYR	6.6
1	O	93	MET	6.5
2	N	213	ALA	6.5
2	P	181	ILE	6.5
1	O	185	ILE	6.5
1	I	68	LEU	6.5
2	P	225	LEU	6.5
1	O	21	ALA	6.5
1	K	38	GLU	6.5
1	I	84	TRP	6.4
1	K	87	VAL	6.4
2	N	264	THR	6.4
2	N	248	VAL	6.4
2	P	221	VAL	6.4
1	O	11	TYR	6.4
2	L	267	ASN	6.4
2	L	213	ALA	6.4
1	I	158	GLY	6.4
1	I	21	ALA	6.3
1	I	85	MET	6.3
1	M	85	MET	6.3
2	N	166	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	O	198	PRO	6.3
2	N	170	VAL	6.3
1	I	103	LEU	6.3
1	O	33	ILE	6.3
1	M	103	LEU	6.3
2	L	119	ALA	6.3
1	I	96	SER	6.3
2	N	169	THR	6.2
1	K	74	GLN	6.2
2	N	263	VAL	6.2
1	K	136	SER	6.2
1	I	56	ALA	6.2
1	M	167	VAL	6.2
1	K	181	ALA	6.2
1	I	172	GLU	6.2
1	O	47	ARG	6.2
2	L	269	GLN	6.2
2	L	166	ARG	6.2
2	P	219	GLN	6.1
1	M	29	SER	6.1
1	O	85	MET	6.1
2	J	22	VAL	6.1
1	O	158	GLY	6.1
1	O	179	SER	6.1
1	I	19	GLN	6.1
1	O	4	LEU	6.1
2	N	223	VAL	6.1
1	C	178	PRO	6.1
1	I	136	SER	6.1
1	O	70	ALA	6.1
2	J	273	GLY	6.1
1	O	106	ALA	6.1
1	M	170	MET	6.1
2	L	230	THR	6.1
1	M	51	THR	6.0
2	L	214	SER	6.0
1	K	194	GLY	6.0
1	K	177	LEU	6.0
1	O	143	ILE	6.0
2	J	214	SER	6.0
1	M	33	ILE	6.0
1	M	140	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
2	L	120	ILE	6.0
2	L	126	ILE	6.0
2	N	22	VAL	6.0
1	M	177	LEU	6.0
1	O	137	ALA	6.0
1	I	71	THR	6.0
2	L	229	GLY	5.9
1	M	106	ALA	5.9
2	L	225	LEU	5.9
2	J	261	GLY	5.9
2	L	67	VAL	5.9
2	P	207	SER	5.9
2	L	266	GLY	5.9
1	K	10	ILE	5.8
1	I	87	VAL	5.8
1	K	152	VAL	5.8
1	I	11	TYR	5.8
2	N	182	PRO	5.8
2	L	175	TYR	5.8
1	M	180	ASP	5.8
1	M	34	GLN	5.8
2	J	20	VAL	5.8
2	P	20	VAL	5.8
1	O	83	PHE	5.8
2	J	181	ILE	5.8
1	K	172	GLU	5.8
1	M	143	ILE	5.8
1	K	179	SER	5.8
2	N	188	ALA	5.7
1	O	34	GLN	5.7
1	K	70	ALA	5.7
1	K	166	LEU	5.7
2	L	215	PHE	5.7
1	K	33	ILE	5.7
1	M	165	ALA	5.7
1	K	85	MET	5.7
1	M	160	ARG	5.7
2	N	212	THR	5.7
2	N	178	SER	5.7
1	M	66	ARG	5.7
2	L	210	THR	5.7
1	O	203	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	P	170	VAL	5.7
1	K	11	TYR	5.6
1	K	7	THR	5.6
1	O	176	LYS	5.6
1	K	21	ALA	5.6
1	I	70	ALA	5.6
1	K	176	LYS	5.5
1	K	114	TYR	5.5
1	M	138	ASN	5.5
2	L	211	ASN	5.5
2	P	210	THR	5.5
2	P	260	GLY	5.5
2	P	223	VAL	5.5
1	K	54	LEU	5.5
1	O	140	LEU	5.5
1	K	148	TYR	5.5
2	P	266	GLY	5.5
1	M	7	THR	5.5
2	N	116	GLY	5.5
1	O	142	LEU	5.4
2	P	262	GLN	5.4
1	K	203	VAL	5.4
2	P	166	ARG	5.4
2	N	18	ALA	5.4
1	M	53	PRO	5.4
2	L	170	VAL	5.4
2	L	207	SER	5.4
2	P	267	ASN	5.4
1	O	178	PRO	5.3
1	M	68	LEU	5.3
1	I	106	ALA	5.3
1	I	167	VAL	5.3
1	K	116	ARG	5.3
2	J	222	GLY	5.3
1	M	200	MET	5.3
1	M	90	ILE	5.3
2	L	53	THR	5.3
2	L	124	SER	5.3
2	J	272	ILE	5.3
1	K	90	ILE	5.3
1	I	198	PRO	5.3
1	K	29	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	K	155	LEU	5.2
1	I	177	LEU	5.2
1	K	167	VAL	5.2
2	N	230	THR	5.2
1	O	148	TYR	5.2
2	N	225	LEU	5.2
1	O	101	ASN	5.2
1	M	5	GLY	5.2
2	L	20	VAL	5.2
1	I	200	MET	5.1
1	K	142	LEU	5.1
2	P	169	THR	5.1
2	J	115	ALA	5.1
2	L	260	GLY	5.1
2	P	174	ASP	5.1
2	P	53	THR	5.1
1	K	160	ARG	5.1
1	M	136	SER	5.1
2	L	273	GLY	5.1
2	J	210	THR	5.1
1	I	47	ARG	5.1
1	K	120	LEU	5.1
1	M	96	SER	5.1
1	O	92	SER	5.0
1	O	131	LEU	5.0
2	N	209	PHE	5.0
1	O	9	VAL	5.0
1	M	74	GLN	5.0
2	J	260	GLY	5.0
1	I	176	LYS	5.0
1	K	151	THR	5.0
1	M	171	GLY	5.0
1	K	6	ALA	5.0
1	I	36	TRP	5.0
1	I	179	SER	5.0
1	O	167	VAL	5.0
2	L	252	LEU	5.0
1	K	132	ARG	5.0
1	I	54	LEU	4.9
1	K	64	THR	4.9
1	M	157	ALA	4.9
1	M	129	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
2	J	211	ASN	4.9
1	K	53	PRO	4.9
1	I	165	ALA	4.9
2	N	242	ALA	4.9
1	M	4	LEU	4.9
2	P	168	VAL	4.9
2	N	199	GLY	4.8
1	I	181	ALA	4.8
1	O	19	GLN	4.8
1	O	180	ASP	4.8
1	K	126	GLN	4.8
1	K	196	LEU	4.8
1	K	31	TYR	4.8
1	O	74	GLN	4.8
2	N	233	PRO	4.8
1	O	97	LYS	4.8
2	J	219	GLN	4.8
2	L	150	ALA	4.8
1	M	35	SER	4.8
1	K	186	THR	4.8
1	I	137	ALA	4.7
2	N	24	LEU	4.7
2	P	115	ALA	4.7
2	J	148	ILE	4.7
1	K	47	ARG	4.7
2	P	22	VAL	4.7
1	I	185	ILE	4.7
1	I	105	LEU	4.7
1	K	16	LYS	4.7
2	L	148	ILE	4.7
1	M	172	GLU	4.7
2	J	207	SER	4.7
1	M	99	THR	4.7
1	K	91	PRO	4.7
2	J	216	SER	4.7
2	N	269	GLN	4.7
2	P	104	PRO	4.7
2	L	257	ALA	4.7
1	K	66	ARG	4.7
1	M	31	TYR	4.7
2	P	264	THR	4.7
1	O	49	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	M	173	SER	4.6
1	M	9	VAL	4.6
1	M	84	TRP	4.6
1	I	34	GLN	4.6
2	N	53	THR	4.6
2	N	229	GLY	4.6
2	N	148	ILE	4.6
1	O	170	MET	4.6
2	J	15	GLY	4.6
1	M	54	LEU	4.6
1	M	83	PHE	4.6
1	I	116	ARG	4.5
1	M	92	SER	4.5
1	K	119	LYS	4.5
1	M	36	TRP	4.5
2	L	217	PRO	4.5
1	K	109	SER	4.5
1	O	152	VAL	4.5
1	O	151	THR	4.5
1	M	120	LEU	4.5
1	K	158	GLY	4.5
2	J	267	ASN	4.5
2	N	257	ALA	4.5
2	J	166	ARG	4.5
1	I	50	VAL	4.5
2	N	259	THR	4.5
1	G	178	PRO	4.5
1	M	145	PRO	4.5
1	I	143	ILE	4.5
2	P	273	GLY	4.5
1	I	6	ALA	4.5
2	L	104	PRO	4.4
1	I	10	ILE	4.4
2	J	124	SER	4.4
1	K	58	LYS	4.4
1	K	117	PRO	4.4
2	L	129	LEU	4.4
2	P	28	VAL	4.4
1	O	122	LEU	4.4
1	I	160	ARG	4.4
2	L	218	ALA	4.4
2	L	174	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	O	99	THR	4.4
1	O	187	TYR	4.4
1	K	56	ALA	4.4
2	L	18	ALA	4.4
1	O	114	TYR	4.4
2	L	250	LEU	4.4
1	I	99	THR	4.4
1	M	121	ALA	4.4
1	K	24	ASN	4.4
2	N	197	LEU	4.3
2	N	201	THR	4.3
1	O	53	PRO	4.3
2	N	217	PRO	4.3
1	K	100	GLU	4.3
2	L	185	VAL	4.3
1	O	200	MET	4.3
2	L	15	GLY	4.3
1	O	116	ARG	4.3
1	I	120	LEU	4.3
1	I	132	ARG	4.3
1	I	121	ALA	4.3
1	I	122	LEU	4.3
2	L	245	THR	4.3
1	M	79	ARG	4.3
2	P	177	GLY	4.3
1	K	122	LEU	4.3
2	N	258	ARG	4.3
1	G	177	LEU	4.3
1	K	140	LEU	4.3
2	P	175	TYR	4.3
1	K	99	THR	4.3
2	P	148	ILE	4.3
1	I	9	VAL	4.3
1	K	171	GLY	4.2
1	K	187	TYR	4.2
1	M	117	PRO	4.2
1	O	172	GLU	4.2
2	L	191	GLN	4.2
2	N	124	SER	4.2
2	N	228	ASN	4.2
2	L	278	TYR	4.2
2	L	221	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	178	PRO	4.2
1	O	165	ALA	4.2
1	K	121	ALA	4.2
1	I	37	VAL	4.2
1	I	173	SER	4.2
1	K	84	TRP	4.2
2	J	270	SER	4.2
2	N	177	GLY	4.2
1	K	198	PRO	4.2
1	I	31	TYR	4.2
2	L	115	ALA	4.2
1	I	8	ARG	4.2
1	M	45	ASP	4.2
2	P	230	THR	4.1
1	I	187	TYR	4.1
1	I	203	VAL	4.1
1	K	159	THR	4.1
2	P	191	GLN	4.1
1	O	121	ALA	4.1
1	M	17	GLN	4.1
2	J	279	GLN	4.1
1	M	6	ALA	4.1
2	N	262	GLN	4.1
1	O	90	ILE	4.1
2	J	150	ALA	4.1
1	I	166	LEU	4.1
1	M	37	VAL	4.1
2	N	195	TYR	4.1
2	J	232	ILE	4.0
1	K	82	LEU	4.0
1	O	68	LEU	4.0
1	K	199	LYS	4.0
2	N	221	VAL	4.0
1	K	180	ASP	4.0
2	P	257	ALA	4.0
1	M	166	LEU	4.0
1	M	187	TYR	4.0
2	N	42	ILE	4.0
1	K	57	MET	4.0
1	M	186	THR	4.0
2	B	172	LEU	4.0
2	L	33	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
2	J	240	LEU	4.0
1	M	131	LEU	4.0
2	P	172	LEU	4.0
2	L	167	ASP	4.0
1	K	123	PRO	4.0
2	P	196	TYR	4.0
1	M	158	GLY	4.0
2	L	24	LEU	4.0
1	M	168	PRO	3.9
1	M	49	ILE	3.9
1	K	189	THR	3.9
2	F	172	LEU	3.9
1	O	109	SER	3.9
1	K	192	ASP	3.9
1	M	192	ASP	3.9
1	M	199	LYS	3.9
1	I	161	VAL	3.9
2	N	254	ALA	3.9
2	N	203	ASP	3.9
1	M	10	ILE	3.9
2	L	28	VAL	3.9
2	N	234	ALA	3.9
1	K	143	ILE	3.9
2	L	42	ILE	3.9
1	O	51	THR	3.9
2	N	278	TYR	3.9
2	H	215	PHE	3.9
2	N	115	ALA	3.9
1	K	79	ARG	3.9
1	K	202	GLY	3.9
1	M	189	THR	3.9
2	L	212	THR	3.9
1	I	138	ASN	3.9
1	M	132	ARG	3.9
2	J	118	VAL	3.9
2	F	215	PHE	3.9
2	N	249	SER	3.9
1	M	176	LYS	3.9
2	P	36	VAL	3.9
1	O	160	ARG	3.9
1	M	109	SER	3.9
2	J	137	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	232	ILE	3.8
2	J	255	ASN	3.8
2	N	176	PRO	3.8
1	O	8	ARG	3.8
2	N	250	LEU	3.8
1	I	114	TYR	3.8
1	M	2	VAL	3.8
2	J	258	ARG	3.8
1	I	152	VAL	3.8
2	L	93	VAL	3.8
2	N	216	SER	3.8
2	J	254	ALA	3.8
1	O	27	GLU	3.8
1	O	58	LYS	3.8
1	I	115	TYR	3.8
1	K	129	GLU	3.8
2	J	169	THR	3.8
2	N	239	SER	3.8
2	P	193	LEU	3.8
1	K	190	ILE	3.7
2	J	53	THR	3.7
2	N	210	THR	3.7
2	P	120	ILE	3.7
1	M	27	GLU	3.7
1	O	66	ARG	3.7
1	I	74	GLN	3.7
2	D	172	LEU	3.7
1	O	72	ASN	3.7
1	O	22	VAL	3.7
2	N	36	VAL	3.7
2	N	243	VAL	3.7
1	I	32	LEU	3.7
1	K	49	ILE	3.7
1	K	112	LYS	3.7
2	J	30	VAL	3.7
1	M	122	LEU	3.7
1	I	159	THR	3.7
1	M	21	ALA	3.7
1	I	129	GLU	3.7
1	K	17	GLN	3.7
1	K	22	VAL	3.7
1	O	23	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	O	57	MET	3.7
1	I	125	ASP	3.6
2	N	189	LYS	3.6
2	J	263	VAL	3.6
2	N	112	VAL	3.6
1	O	107	ILE	3.6
2	N	255	ASN	3.6
2	L	146	TRP	3.6
1	O	17	GLN	3.6
1	O	186	THR	3.6
1	O	157	ALA	3.6
1	M	163	GLU	3.6
2	L	224	GLN	3.6
1	K	161	VAL	3.6
1	I	100	GLU	3.6
1	M	164	ASN	3.6
2	J	67	VAL	3.6
1	A	93	MET	3.5
1	O	6	ALA	3.5
2	N	191	GLN	3.5
1	A	161	VAL	3.5
1	I	22	VAL	3.5
1	A	178	PRO	3.5
1	O	100	GLU	3.5
2	N	137	TYR	3.5
1	K	88	LYS	3.5
1	M	130	LYS	3.5
2	J	174	ASP	3.5
2	J	252	LEU	3.5
1	M	15	GLN	3.5
2	J	157	PRO	3.5
2	P	33	ASN	3.5
2	L	106	ALA	3.5
1	K	169	PRO	3.5
1	M	198	PRO	3.5
2	L	179	VAL	3.5
2	N	200	THR	3.5
2	N	245	THR	3.5
2	N	231	ILE	3.5
1	K	78	ASP	3.5
2	P	186	TYR	3.5
1	A	177	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	172	LEU	3.5
1	M	16	LYS	3.5
1	O	155	LEU	3.5
2	L	183	LEU	3.5
2	N	277	VAL	3.5
1	I	109	SER	3.4
2	L	80	SER	3.4
1	M	196	LEU	3.4
1	I	16	LYS	3.4
1	M	20	LEU	3.4
1	O	89	ALA	3.4
2	P	232	ILE	3.4
1	O	166	LEU	3.4
1	O	199	LYS	3.4
2	N	279	GLN	3.4
2	J	278	TYR	3.4
2	L	244	GLY	3.4
1	O	119	LYS	3.4
2	P	265	ALA	3.4
2	D	215	PHE	3.4
1	K	73	ASN	3.4
2	N	33	ASN	3.4
1	K	113	LEU	3.4
1	M	64	THR	3.4
1	I	38	GLU	3.4
1	M	50	VAL	3.4
2	P	195	TYR	3.3
1	M	38	GLU	3.3
2	J	191	GLN	3.3
1	I	82	LEU	3.3
2	N	183	LEU	3.3
2	N	16	GLY	3.3
1	O	32	LEU	3.3
1	M	125	ASP	3.3
2	L	216	SER	3.3
2	N	244	GLY	3.3
1	M	119	LYS	3.3
1	O	64	THR	3.3
2	L	264	THR	3.3
2	L	255	ASN	3.3
1	I	119	LYS	3.3
2	J	116	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	P	116	GLY	3.3
2	L	248	VAL	3.3
1	I	199	LYS	3.3
1	M	30	THR	3.3
2	P	255	ASN	3.3
1	M	112	LYS	3.3
2	N	108	TYR	3.3
1	K	5	GLY	3.3
1	K	111	ILE	3.3
1	M	202	GLY	3.3
1	O	78	ASP	3.3
2	L	54	ASP	3.3
1	O	189	THR	3.3
2	J	250	LEU	3.3
2	P	137	TYR	3.3
1	I	2	VAL	3.2
1	I	53	PRO	3.2
1	I	196	LEU	3.2
2	L	137	TYR	3.2
1	O	38	GLU	3.2
1	I	64	THR	3.2
2	D	165	ALA	3.2
2	P	250	LEU	3.2
1	K	2	VAL	3.2
2	H	165	ALA	3.2
2	N	265	ALA	3.2
1	O	138	ASN	3.2
2	L	22	VAL	3.2
2	N	163	VAL	3.2
1	I	79	ARG	3.2
1	I	180	ASP	3.2
2	J	120	ILE	3.2
2	N	146	TRP	3.2
1	K	8	ARG	3.2
2	J	146	TRP	3.2
1	O	194	GLY	3.2
2	N	15	GLY	3.2
2	P	258	ARG	3.2
2	L	263	VAL	3.2
2	J	104	PRO	3.2
2	N	167	ASP	3.2
1	I	189	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	242	ALA	3.2
1	I	23	THR	3.1
1	O	197	THR	3.1
2	N	237	THR	3.1
2	J	126	ILE	3.1
2	J	170	VAL	3.1
2	L	279	GLN	3.1
2	J	178	SER	3.1
1	C	72	ASN	3.1
2	N	52	ILE	3.1
2	L	144	PHE	3.1
2	P	204	ALA	3.1
1	G	176	LYS	3.1
1	K	168	PRO	3.1
1	O	54	LEU	3.1
1	I	66	ARG	3.1
1	I	30	THR	3.1
1	I	81	SER	3.1
1	O	196	LEU	3.1
2	P	178	SER	3.1
1	G	158	GLY	3.1
2	H	261	GLY	3.1
1	M	62	GLU	3.1
2	L	276	PHE	3.1
1	E	178	PRO	3.1
2	J	168	VAL	3.1
2	J	230	THR	3.1
1	M	32	LEU	3.1
2	N	173	PRO	3.1
2	L	123	GLY	3.1
2	N	14	GLY	3.1
2	P	234	ALA	3.1
2	N	123	GLY	3.1
1	M	111	ILE	3.1
1	K	139	SER	3.0
2	L	187	CYS	3.0
1	I	140	LEU	3.0
1	M	114	TYR	3.0
2	N	205	GLY	3.0
2	P	236	ASN	3.0
1	C	160	ARG	3.0
1	K	30	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	24	LEU	3.0
2	L	169	THR	3.0
1	I	58	LYS	3.0
2	J	163	VAL	3.0
1	M	8	ARG	3.0
1	M	190	ILE	3.0
2	L	258	ARG	3.0
2	N	187	CYS	3.0
1	K	51	THR	3.0
1	I	27	GLU	3.0
1	M	126	GLN	3.0
2	L	61	GLY	3.0
2	J	236	ASN	3.0
2	P	67	VAL	3.0
1	I	92	SER	2.9
2	J	183	LEU	2.9
2	L	68	LEU	2.9
2	N	104	PRO	2.9
2	N	193	LEU	2.9
1	M	161	VAL	2.9
1	M	175	VAL	2.9
1	O	26	ASP	2.9
2	J	186	TYR	2.9
1	C	132	ARG	2.9
1	K	134	ARG	2.9
2	J	47	ASP	2.9
2	H	175	TYR	2.9
2	B	215	PHE	2.9
2	P	109	LEU	2.9
2	L	163	VAL	2.9
2	N	238	VAL	2.9
2	J	119	ALA	2.9
1	M	149	TYR	2.9
1	I	171	GLY	2.9
2	L	195	TYR	2.9
1	A	140	LEU	2.9
2	N	276	PHE	2.9
2	P	182	PRO	2.9
1	M	22	VAL	2.9
2	L	118	VAL	2.9
1	M	73	ASN	2.9
2	L	186	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	P	240	LEU	2.9
1	I	194	GLY	2.9
2	J	28	VAL	2.9
1	A	176	LYS	2.9
2	L	204	ALA	2.9
2	J	80	SER	2.9
1	K	12	PRO	2.8
1	M	97	LYS	2.8
2	D	171	THR	2.8
2	P	30	VAL	2.8
2	P	259	THR	2.8
1	K	23	THR	2.8
2	J	93	VAL	2.8
2	J	221	VAL	2.8
1	I	156	ASN	2.8
1	O	63	ASN	2.8
2	L	47	ASP	2.8
1	M	19	GLN	2.8
2	L	262	GLN	2.8
2	N	126	ILE	2.8
2	P	126	ILE	2.8
2	D	175	TYR	2.8
2	L	277	VAL	2.8
1	O	173	SER	2.8
2	P	176	PRO	2.8
2	P	54	ASP	2.8
2	P	24	LEU	2.8
1	I	178	PRO	2.8
2	L	157	PRO	2.8
1	K	204	MET	2.8
2	J	195	TYR	2.8
2	N	21	TYR	2.8
1	O	29	SER	2.8
2	J	18	ALA	2.8
2	J	33	ASN	2.8
1	E	176	LYS	2.8
2	P	269	GLN	2.8
1	O	175	VAL	2.7
2	F	175	TYR	2.7
2	N	149	TYR	2.7
2	P	248	VAL	2.7
2	P	18	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	142	LEU	2.7
2	L	172	LEU	2.7
2	N	120	ILE	2.7
1	K	141	THR	2.7
2	N	171	THR	2.7
1	I	46	GLY	2.7
2	J	266	GLY	2.7
1	O	60	LYS	2.7
1	O	161	VAL	2.7
2	L	127	ALA	2.7
2	N	180	PRO	2.7
1	I	72	ASN	2.7
1	M	139	SER	2.7
2	P	163	VAL	2.7
1	K	149	TYR	2.7
1	M	58	LYS	2.7
2	L	209	PHE	2.7
2	N	157	PRO	2.7
1	M	159	THR	2.7
1	O	202	GLY	2.7
2	L	261	GLY	2.7
2	N	185	VAL	2.7
1	K	145	PRO	2.7
2	L	102	PRO	2.7
1	G	135	ARG	2.7
1	O	10	ILE	2.7
1	O	79	ARG	2.7
2	N	54	ASP	2.7
2	L	36	VAL	2.7
1	I	134	ARG	2.7
1	M	57	MET	2.7
1	O	73	ASN	2.7
1	C	1	GLY	2.7
1	M	14	GLY	2.7
2	P	171	THR	2.7
1	I	97	LYS	2.7
1	O	31	TYR	2.6
2	P	278	TYR	2.6
1	G	140	LEU	2.6
1	I	113	LEU	2.6
2	N	252	LEU	2.6
2	L	162	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	J	229	GLY	2.6
2	N	251	GLY	2.6
2	N	204	ALA	2.6
1	M	82	LEU	2.6
2	N	206	ASN	2.6
2	P	1	PHE	2.6
1	K	61	LYS	2.6
2	P	199	GLY	2.6
1	M	193	TYR	2.6
1	O	113	LEU	2.6
1	M	72	ASN	2.6
1	O	112	LYS	2.6
2	N	1	PHE	2.6
2	J	193	LEU	2.6
2	J	220	GLY	2.6
2	L	16	GLY	2.6
1	I	49	ILE	2.6
2	J	42	ILE	2.6
1	M	56	ALA	2.6
1	I	155	LEU	2.6
1	O	62	GLU	2.6
2	P	249	SER	2.6
2	D	166	ARG	2.6
1	K	63	ASN	2.6
1	M	26	ASP	2.6
1	M	60	LYS	2.6
1	I	107	ILE	2.6
2	L	52	ILE	2.6
1	K	27	GLU	2.6
2	P	93	VAL	2.6
2	L	125	LEU	2.5
1	K	130	LYS	2.5
2	P	185	VAL	2.5
2	N	190	SER	2.5
2	P	108	TYR	2.5
1	K	60	LYS	2.5
1	K	175	VAL	2.5
2	N	150	ALA	2.5
1	I	91	PRO	2.5
1	O	159	THR	2.5
1	I	1	GLY	2.5
1	K	89	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	52	PRO	2.5
1	O	3	ALA	2.5
2	J	203	ASP	2.5
2	L	228	ASN	2.5
2	J	264	THR	2.5
1	O	204	MET	2.5
1	G	162	LEU	2.5
1	A	132	ARG	2.5
2	J	102	PRO	2.5
1	K	118	ALA	2.5
1	C	182	GLY	2.5
2	J	16	GLY	2.5
1	I	108	ILE	2.5
1	K	50	VAL	2.5
1	G	98	LEU	2.4
1	O	132	ARG	2.4
2	L	240	LEU	2.4
2	L	49	PRO	2.4
2	L	176	PRO	2.4
1	K	25	ASN	2.4
1	O	117	PRO	2.4
1	K	15	GLN	2.4
2	P	47	ASP	2.4
1	I	175	VAL	2.4
1	O	56	ALA	2.4
1	M	78	ASP	2.4
2	J	167	ASP	2.4
2	P	253	THR	2.4
1	G	155	LEU	2.4
1	I	90	ILE	2.4
2	L	95	TYR	2.4
1	M	23	THR	2.4
1	K	3	ALA	2.4
2	F	165	ALA	2.4
2	P	119	ALA	2.4
1	C	135	ARG	2.4
1	M	134	ARG	2.4
1	M	204	MET	2.4
2	P	209	PHE	2.4
1	M	86	ASN	2.4
2	N	7	ASN	2.4
2	L	254	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	252	LEU	2.4
1	K	1	GLY	2.4
1	K	131	LEU	2.4
2	J	125	LEU	2.4
1	G	1	GLY	2.4
1	O	126	GLN	2.4
1	O	36	TRP	2.4
1	K	163	GLU	2.4
2	J	54	ASP	2.4
1	A	179	SER	2.4
2	J	11	ILE	2.3
1	G	72	ASN	2.3
2	N	164	SER	2.3
1	M	3	ALA	2.3
2	B	165	ALA	2.3
2	J	127	ALA	2.3
2	L	208	ILE	2.3
1	G	205	GLU	2.3
2	P	14	GLY	2.3
2	P	183	LEU	2.3
2	J	248	VAL	2.3
2	N	28	VAL	2.3
1	O	123	PRO	2.3
2	J	182	PRO	2.3
2	J	1	PHE	2.3
2	L	48	TYR	2.3
2	L	103	TRP	2.3
2	N	240	LEU	2.3
1	G	167	VAL	2.3
2	P	173	PRO	2.3
1	M	24	ASN	2.3
2	N	50	GLU	2.3
1	O	182	GLY	2.3
2	N	10	ALA	2.3
1	K	110	ARG	2.3
2	J	176	PRO	2.3
2	L	173	PRO	2.3
2	P	279	GLN	2.3
1	K	14	GLY	2.3
1	E	140	LEU	2.3
1	O	108	ILE	2.3
2	N	47	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	62	GLU	2.3
2	J	7	ASN	2.3
2	N	246	SER	2.3
1	O	61	LYS	2.3
2	J	242	ALA	2.3
1	M	107	ILE	2.3
2	N	117	GLY	2.3
1	A	157	ALA	2.2
1	I	3	ALA	2.2
2	N	27	VAL	2.2
1	O	25	ASN	2.2
1	C	176	LYS	2.2
1	G	160	ARG	2.2
2	P	164	SER	2.2
2	D	167	ASP	2.2
1	E	160	ARG	2.2
1	C	129	GLU	2.2
1	M	154	GLU	2.2
2	P	103	TRP	2.2
2	N	125	LEU	2.2
2	N	37	ASP	2.2
2	L	231	ILE	2.2
1	O	171	GLY	2.2
1	C	177	LEU	2.2
1	K	97	LYS	2.2
2	L	109	LEU	2.2
1	M	43	VAL	2.2
1	I	26	ASP	2.2
1	C	93	MET	2.2
2	P	245	THR	2.2
1	K	28	ASN	2.2
2	N	274	VAL	2.2
1	I	202	GLY	2.2
2	N	273	GLY	2.2
1	M	61	LYS	2.2
1	M	194	GLY	2.2
2	L	117	GLY	2.2
2	B	164	SER	2.2
2	L	193	LEU	2.2
2	N	129	LEU	2.2
1	M	89	ALA	2.2
2	J	277	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	183	SER	2.2
1	M	44	LYS	2.2
2	J	172	LEU	2.2
2	P	131	LEU	2.2
2	L	86	THR	2.1
2	N	30	VAL	2.1
2	J	78	SER	2.1
1	M	110	ARG	2.1
2	L	37	ASP	2.1
2	L	197	LEU	2.1
1	I	73	ASN	2.1
2	J	185	VAL	2.1
1	E	135	ARG	2.1
2	N	109	LEU	2.1
1	K	153	THR	2.1
2	P	200	THR	2.1
1	I	89	ALA	2.1
2	J	234	ALA	2.1
2	N	247	ALA	2.1
1	A	135	ARG	2.1
1	K	124	PRO	2.1
2	N	48	TYR	2.1
2	N	67	VAL	2.1
2	P	48	TYR	2.1
1	I	190	ILE	2.1
1	O	139	SER	2.1
1	E	98	LEU	2.1
1	O	120	LEU	2.1
1	G	159	THR	2.1
1	O	153	THR	2.1
2	L	60	ARG	2.1
2	N	119	ALA	2.1
2	P	254	ALA	2.1
1	M	123	PRO	2.1
1	K	107	ILE	2.1
1	K	108	ILE	2.1
1	E	177	LEU	2.1
2	L	76	LYS	2.1
2	P	220	GLY	2.1
1	G	132	ARG	2.1
2	J	171	THR	2.1
2	N	103	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	217	PRO	2.1
2	B	167	ASP	2.1
2	N	130	ILE	2.1
2	J	269	GLN	2.1
1	O	5	GLY	2.1
2	L	220	GLY	2.1
1	G	93	MET	2.1
1	K	115	TYR	2.1
2	B	175	TYR	2.1
2	J	162	ASP	2.1
2	B	171	THR	2.1
1	O	88	LYS	2.1
2	L	247	ALA	2.1
2	N	4	LYS	2.1
1	I	192	ASP	2.1
1	K	125	ASP	2.1
1	M	169	PRO	2.1
2	J	187	CYS	2.1
1	O	16	LYS	2.0
1	M	197	THR	2.0
1	I	17	GLN	2.0
2	L	130	ILE	2.0
1	O	75	LEU	2.0
1	A	205	GLU	2.0
1	M	118	ALA	2.0
1	I	112	LYS	2.0
1	M	1	GLY	2.0
1	O	44	LYS	2.0
1	C	142	LEU	2.0
2	P	206	ASN	2.0
1	O	163	GLU	2.0
2	J	245	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MAN	P	1607	12/12	0.26	0.08	110,112,116,117	0
3	MAN	D	1601	12/12	0.18	0.07	28,36,41,41	0
3	MAN	F	1502	12/12	0.18	-0.00	29,35,41,41	0
3	MAN	H	1603	12/12	0.16	-0.10	28,34,39,39	0
3	MAN	J	1605	12/12	0.25	-0.28	96,100,105,106	0
3	MAN	B	1500	12/12	0.15	-0.81	30,35,39,39	0
3	MAN	L	1504	12/12	0.23	-0.92	96,99,103,106	0
3	MAN	N	1506	12/12	0.18	-1.15	90,94,100,101	0

6.5 Other polymers

There are no such residues in this entry.